

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of glycine with formaldehyde to give **serine** in the  
presence of copper-based catalysts in neutral aqueous solution)

IT 7447-39-4, Copper dichloride, uses  
RL: CAT (Catalyst use); USES (Uses)  
(preparation of copper complexes as catalysts for the reaction of glycine  
with formaldehyde to give **serine** in neutral aqueous solution)

IT 460730-91-0P 460730-92-1P 460730-93-2P 460730-94-3P  
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);  
USES (Uses)  
(preparation of copper complexes as catalysts for the reaction of glycine  
with formaldehyde to give **serine** in neutral aqueous solution)

IT 623-24-5, 1,4-Bis(bromomethyl)benzene 626-15-3, 1,3-  
Bis(bromomethyl)benzene 1539-42-0, Bis(2-pyridylmethyl)amine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of copper complexes as catalysts for the reaction of glycine  
with formaldehyde to give **serine** in neutral aqueous solution)

IT 460357-04-4P 460357-05-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of copper complexes as catalysts for the reaction of glycine  
with formaldehyde to give **serine** in neutral aqueous solution)

IT 17149-11-0P  
RL: BYP (Byproduct); PREP (Preparation)  
(reaction of glycine with formaldehyde to give **serine** in the  
presence of copper-based catalysts in neutral aqueous solution)

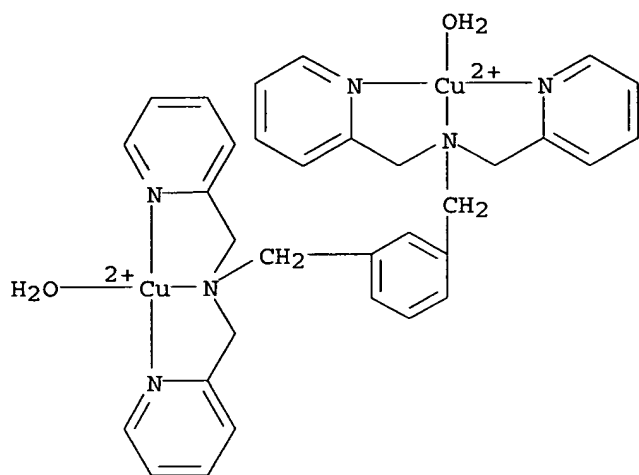
IT 50-00-0, Formaldehyde, reactions 56-40-6, Glycine, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of glycine with formaldehyde to give **serine** in the  
presence of copper-based catalysts in neutral aqueous solution)

IT 302-84-1P, **Serine**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(reaction of glycine with formaldehyde to give **serine** in the  
presence of copper-based catalysts in neutral aqueous solution)

IT 460730-92-1P 460730-93-2P  
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);  
USES (Uses)  
(preparation of copper complexes as catalysts for the reaction of glycine  
with formaldehyde to give **serine** in neutral aqueous solution)

RN 460730-92-1 CAPLUS  
CN Copper(4+), diaqua[ $\mu$ -[N,N',N'',N''']-tetrakis[(2-pyridinyl-  
 $\kappa$ N)methyl]-1,3-benzenedimethanamine- $\kappa$ N: $\kappa$ N']]di-,  
tetrachloride (9CI) (CA INDEX NAME)

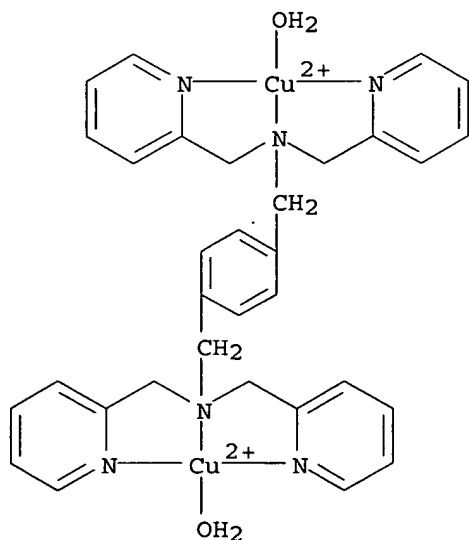
*Considered  
04/28/06  
MCC*



●4 Cl<sup>-</sup>

RN 460730-93-2 CAPLUS

CN Copper(4+), diaqua[μ-[N,N',N'',N'''-tetrakis[(2-pyridinyl-κN)methyl]-1,4-benzenedimethanamine-κN:κN']]di-, tetrachloride (9CI) (CA INDEX NAME)



●4 Cl<sup>-</sup>

IT 460357-04-4P 460357-05-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of copper complexes as catalysts for the reaction of glycine with formaldehyde to give serine in neutral aqueous solution)

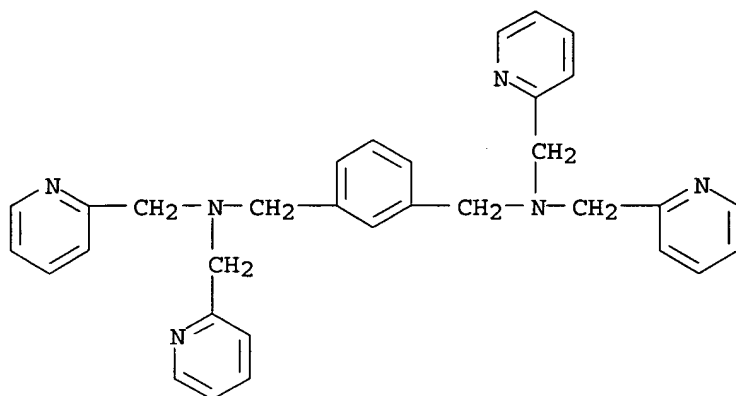
RN 460357-04-4 CAPLUS

CN 1,3-Benzenedimethanamine, N,N,N',N'-tetrakis(2-pyridinylmethyl)-, tetraperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 164298-97-9

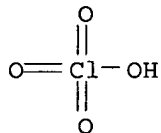
CMF C32 H32 N6



CM 2

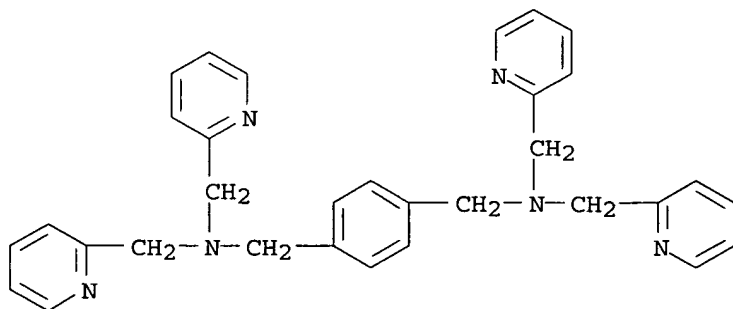
CRN 7601-90-3

CMF Cl H O4



RN 460357-05-5 CAPLUS

CN 1,4-Benzenedimethanamine, N,N,N',N'-tetrakis(2-pyridinylmethyl)-, tetrahydrochloride (9CI) (CA INDEX NAME)



● 4 HCl

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 27 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:51568 CAPLUS  
 DOCUMENT NUMBER: 136:103838  
 TITLE: **Fluorescein**-based metal sensors and their use  
 INVENTOR(S): Lippard, Stephen J.; Burdette, Shawn; Hilderbrand, Scott; Tsien, Roger; Walkup, Grant  
 PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA  
 SOURCE: PCT Int. Appl., 98 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND   | DATE     | APPLICATION NO. | DATE       |
|------------------------|--|----------|-----------------|------------|
| WO 2002004562          | A2   | 20020117 | WO 2001-US41313 | 20010709   |
| WO 2002004562          | A3   | 20020530 |                 |            |
| W:                     | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |            |
| RW:                    | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG   |          |                 |            |
| US 2002106697          | A1   | 20020808 | US 2001-901466  | 20010709   |
| PRIORITY APPLN. INFO.: |  |          | US 2000-216872P | P 20000707 |
|                        |  |          | US 2000-216875P | P 20000707 |
|                        |  |          | US 2001-284384P | P 20010417 |

OTHER SOURCE(S): MARPAT 136:103838  
 AB **Fluorescein**-based ligands are obtained for the detection of metal ions, such as zinc in **intracellular** media. In an example, an orange dye was produced by reductive amination of 4',5'-**fluoresceindicarboxaldehyde** with bis(2-pyridylmethyl)amine and shown to have a Zn-selective **fluorescence** response.  
 IC ICM C09B011-08  
 ICS G01N033-533; G01N033-58  
 CC 41-11 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)  
 Section cross-reference(s): 9, 27, 78, 79, 80  
 ST **fluorescein** based dye prodn zinc **fluorescent** sensor  
**intracellular**  
 IT Crystal structure  
 (preparation and crystal structure of **fluorescein**-based ligand-zinc complex)  
 IT Ligands  
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (production of **fluorescein**-based metal sensors selective for zinc)  
 IT 389625-18-7P  
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (dye; production of **fluorescein**-based metal sensors selective for



zinc)

IT 67567-46-8P 389625-43-8P 389625-45-0P 389625-46-1P 389625-49-4P  
389625-50-7P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate; preparation and crystal structure of **fluorescein**  
-based ligand-zinc complex)

IT 357615-01-1P 357615-02-2P 357615-03-3P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate; production of **fluorescein**-based metal sensors and  
their use)

IT 2513-23-7P 389625-15-4P 389625-16-5P 389625-17-6P 389625-22-3P  
389625-28-9P 389625-29-0P 389625-32-5P 389625-33-6P 389625-34-7P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate; production of **fluorescein**-based metal sensors  
selective for zinc)

IT **357916-12-2P**  
RL: IMF (Industrial manufacture); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)  
(orange dye; production of **fluorescein**-based metal sensors and  
their use)

IT 389625-25-6P  
RL: IMF (Industrial manufacture); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)  
(orange dye; production of **fluorescein**-based metal sensors  
selective for zinc)

IT 67-68-5, DMSO, reactions  
RL: RGT (Reagent); RACT (Reactant or reagent)  
(oxidizing agent; production of **fluorescein**-based metal sensors  
and their use)

IT 389625-41-6P  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation and crystal structure of **fluorescein**-based  
ligand-zinc complex)

IT **389632-92-2P**  
RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)  
(preparation and crystal structure of **fluorescein**-based  
ligand-zinc complex)

IT 7440-66-6, Zinc, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(production of **fluorescein**-based metal sensors selective for  
zinc)

IT 389625-20-1P 389625-21-2P 389625-24-5P  
RL: IMF (Industrial manufacture); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)  
(production of **fluorescein**-based metal sensors selective for  
zinc)

IT **288574-78-7P**  
RL: IMF (Industrial manufacture); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)  
(salmon pink dye; production of **fluorescein**-based metal sensors  
selective for zinc)

IT 1333-74-0, Hydrogen, reactions 5367-32-8, 3-Methyl-4-nitroanisole  
389625-48-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; preparation and crystal structure of **fluorescein**  
-based ligand-zinc complex)

IT 77-48-5 85-44-9, Phthalic anhydride 93-97-0, Benzoic anhydride

608-25-3, 2-Methylresorcinol 1539-42-0, Bis(2-pyridylmethyl)amine  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; production of **fluorescein**-based metal sensors and their use)

IT 62-53-3, Aniline, reactions 127-08-2, Potassium acetate 127-09-3, Sodium acetate 699-83-2 2321-07-5, **Fluorescein** 2491-18-1, L-Methionine methyl ester hydrochloride 2706-56-1, 2-(2-Aminoethyl)pyridine 6201-65-6, 2-Chlororesorcinol 7335-65-1, Hydrazine acetate 7761-88-8, Silver nitrate, reactions 13154-24-0, Triisopropylsilyl chloride 18162-48-6, tert-Butyldimethylsilyl chloride 30525-89-4, Paraformaldehyde 58479-61-1, tert-Butyldiphenylsilyl chloride 65840-40-6, Potassium levulinate 118797-71-0 389625-23-4 389625-31-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; production of **fluorescein**-based metal sensors selective for zinc)

IT 389625-47-2P

RL: IMF (Industrial manufacture); PREP (Preparation)

(yellow dye; preparation and crystal structure of **fluorescein**-based ligand-zinc complex)

IT 389625-19-8P 389625-26-7P 389625-27-8P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(yellow dye; production of **fluorescein**-based metal sensors selective for zinc)

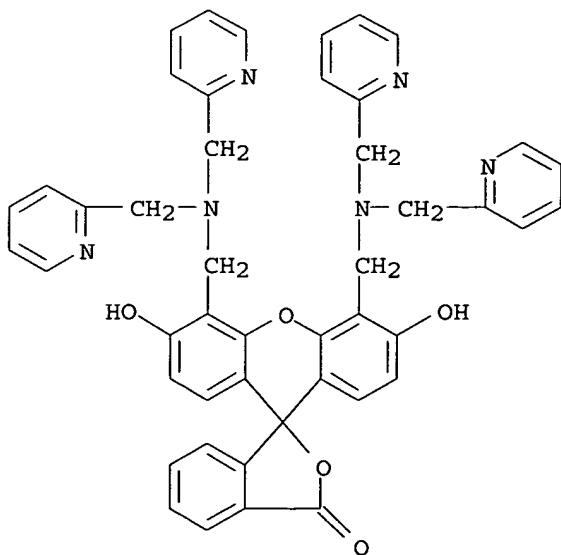
IT 357916-12-2P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(orange dye; production of **fluorescein**-based metal sensors and their use)

RN 357916-12-2 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



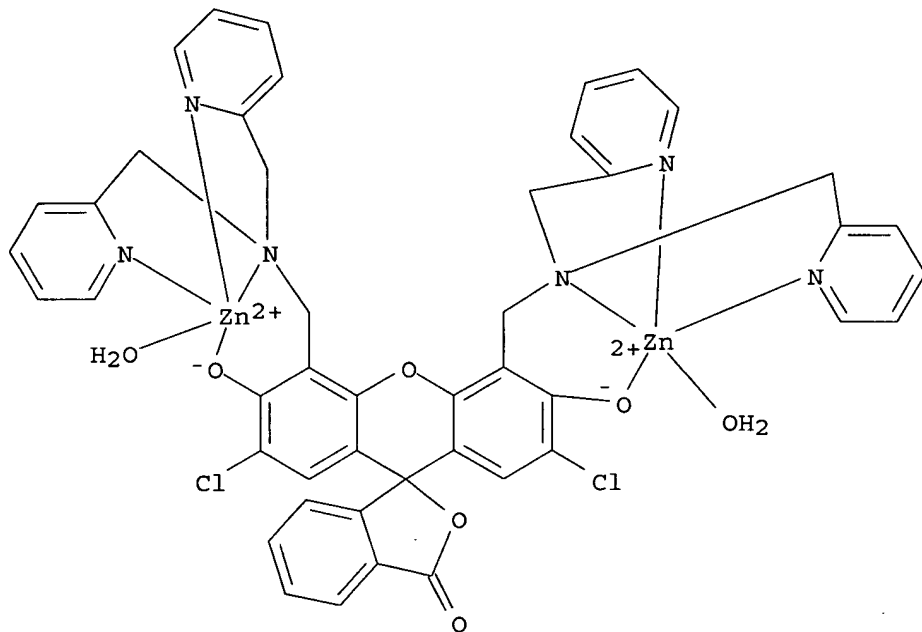
IT 389632-92-2P

RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)  
 (preparation and crystal structure of **fluorescein**-based

ligand-zinc complex)

RN 389632-92-2 CAPLUS

CN Zinc(2+), diaqua[μ-[4',5'-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-2',7'-dichloro-3',6'-di(hydroxy-κO)spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-onato(2-)]di- (9CI)  
(CA INDEX NAME)



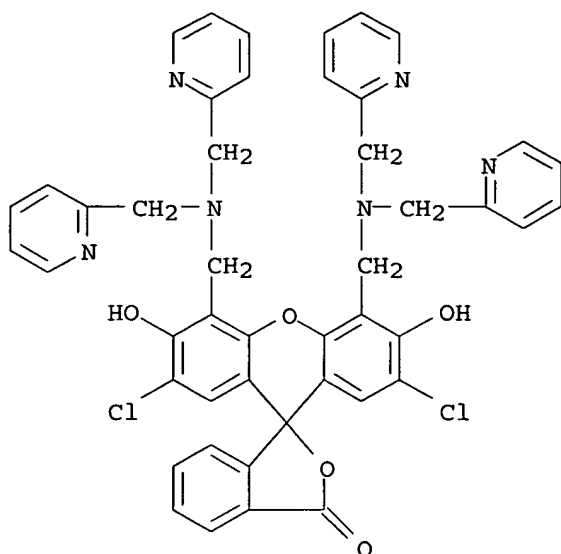
IT 288574-78-7P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(salmon pink dye; production of **fluorescein**-based metal sensors selective for zinc)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



L79 ANSWER 28 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:844893 CAPLUS

DOCUMENT NUMBER: 136:2446

TITLE: Methods for screening molecules using solid phase synthesis with labels

INVENTOR(S): Nova, Michael P.; Potash, Hanan; Xiao, Xiao-yi; Parandoosh, Zahra; David, Gary S.

PATENT ASSIGNEE(S): Discovery Partners International, USA

SOURCE: U.S., 91 pp., Cont.-in-part of U.S. 6,100,026.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 20

PATENT INFORMATION:

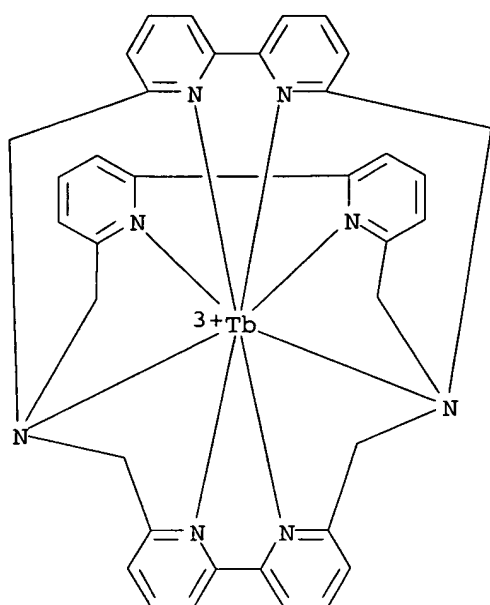
| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| US 6319668  | B1   | 20011120 | US 1996-669252  | 19960624 |
| US 5741462  | A    | 19980421 | US 1995-428662  | 19950425 |
| US 5925562  | A    | 19990720 | US 1995-480196  | 19950607 |
| US 6331273  | B1   | 20011218 | US 1995-473660  | 19950607 |
| US 6352854  | B1   | 20020305 | US 1995-480147  | 19950607 |
| US 6416714  | B1   | 20020709 | US 1995-484486  | 19950607 |
| US 5874214  | A    | 19990223 | US 1995-538387  | 19951003 |
| US 6025129  | A    | 20000215 | US 1995-567746  | 19951205 |
| WO 9636436  | A1   | 19961121 | WO 1996-US6145  | 19960425 |
| W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI |      |          |                 |          |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN  |      |          |                 |          |
| US 6100026  | A    | 20000808 | US 1996-633410  | 19960610 |
| US 6284459  | B1   | 20010904 | US 1996-711426  | 19960905 |
| US 6017496  | A    | 20000125 | US 1996-709435  | 19960906 |
| US 5961923  | A    | 19991005 | US 1996-723423  | 19960930 |

|   |    |          |                 |             |
|---|----|----------|-----------------|-------------|
| WO 9712680  | A2 | 19970410 | WO 1996-US15999 | 19961003    |
| WO 9712680  | A3 | 19970821 |                 |             |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN |    |          |                 |             |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG  |    |          |                 |             |
| AU 9672573  | A1 | 19970428 | AU 1996-72573   | 19961003    |
| EP 853497   | A2 | 19980722 | EP 1996-934064  | 19961003    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI   |    |          |                 |             |
| US 6329139  | B1 | 20011211 | US 1997-912998  | 19970811    |
| US 6340588  | B1 | 20020122 | US 1998-51022   | 19980922    |
| PRIORITY APPLN. INFO.:  |    |          |                 |             |
|   |    |          | US 1995-428662  | A2 19950425 |
|   |    |          | US 1995-473660  | A2 19950607 |
|   |    |          | US 1995-480147  | A2 19950607 |
|   |    |          | US 1995-480196  | A2 19950607 |
|   |    |          | US 1995-484486  | A2 19950607 |
|   |    |          | US 1995-484504  | A2 19950607 |
|   |    |          | US 1995-538387  | A2 19951003 |
|   |    |          | US 1995-567746  | A2 19951205 |
|   |    |          | US 1996-639813  | B2 19960402 |
|   |    |          | WO 1996-US6145  | A2 19960425 |
|   |    |          | US 1996-633410  | A2 19960610 |
|   |    |          | US 1997-945053  | B2 19971021 |
|   |    |          | US 1995-184504  | A2 19950607 |
|   |    |          | US 1996-669252  | A2 19960624 |
|   |    |          | US 1996-711426  | A2 19960905 |
|   |    |          | US 1996-709435  | A2 19960906 |
|   |    |          | US 1996-723423  | A 19960930  |
|   |    |          | WO 1996-US15999 | W 19961003  |
|   |    |          | US 1996-726703  | B2 19961007 |
|   |    |          | US 1996-743984  | A2 19961028 |
|   |    |          | US 1996-741685  | B2 19961031 |
|   |    |          | US 1997-857800  | B2 19970122 |
|   |    |          | US 1997-826253  | B2 19970327 |

AB Combinations, called matrixes with memories, of matrix materials that are encoded with an optically readable code are provided. The matrix materials are those that are used in as supports in solid phase chemical and biochem. syntheses, immunoassays and hybridization reactions. The matrix materials may addnl. include **fluorophores** or other luminescent moieties to produce luminescing matrixes with memories. The memories include electronic and optical storage media and also include optical memories, such as bar codes and other machine-readable codes. By virtue of this combination, mols. and biol. particles, such as phage and viral particles and **cells**, that are in proximity or in phys. contact with the matrix combination can be labeled by programming the memory with identifying information and can be identified by retrieving the stored information. Combinations of matrix materials, memories, and linked mols. and biol. materials are also provided. The combinations have a multiplicity of applications, including combinatorial chemical, isolation and purification of target macromols., capture and detection of macromols. for anal. purposes, selective removal of contaminants, enzymic catalysis, **cell** sorting, drug delivery, chemical modification and other uses. Methods for tagging mols., biol. particles and matrix support materials, immunoassays, receptor binding assays, scintillation proximity assays, non-radioactive proximity assays, and other methods are also provided. Diagrams describing the apparatus are given.

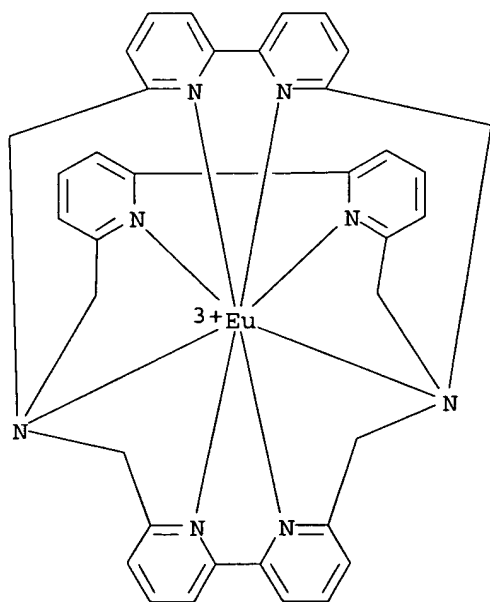
IC ICM C12Q001-68

INCL ICS G01N033-53; C12M001-34; C07H021-04  
 435006000  
 CC 9-1 (Biochemical Methods)  
 Section cross-reference(s): 3, 15  
 IT Analytical apparatus  
 Bar code labels  
 Combinatorial chemistry  
 Combinatorial library  
 Computer program  
 Computers  
 Databases  
 Drug screening  
     **Fluorescent** substances  
 Laboratory ware  
 Luminescence  
 Luminescent substances  
 Memory devices  
 Microtiter plates  
 Optical detectors  
 Optical memory devices  
 Phage display library  
 Protein sequences  
 Radiochemical analysis  
 Recording apparatus  
 Test tubes  
 Vials  
     (methods for screening mols. using solid phase synthesis with labels)  
 IT 81-88-9 92-71-7, 2,5-Diphenyloxazole 120-12-7, Anthracene, uses  
 15082-28-7 60078-97-9, 1-Phenyl-3-mesityl-2-pyrazoline  
 107539-34-4 113031-11-1  
 RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical  
 study); USES (Uses)  
     (methods for screening mols. using solid phase synthesis with labels)  
 IT 7440-21-3, Silicon, analysis 9003-05-8, Polyacrylamide 9003-53-6,  
 Polystyrene 9004-34-6, **Cellulose**, analysis 9012-36-6,  
 Agarose 9017-21-4, Polyvinyltoluene  
 RL: ARU (Analytical role, unclassified); DEV (Device component use); ANST  
 (Analytical study); USES (Uses)  
     (methods for screening mols. using solid phase synthesis with labels)  
 IT 7789-75-5, Calcium **fluoride**, properties 12797-68-1, Yttrium  
 silicate  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
 PROC (Process)  
     (methods for screening mols. using solid phase synthesis with labels)  
 IT 107539-34-4 113031-11-1  
 RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical  
 study); USES (Uses)  
     (methods for screening mols. using solid phase synthesis with labels)  
 RN 107539-34-4 CAPLUS  
 CN Terbiu(m)(3+), (1,14,39,40,41,42,43,44-octaazaocatacyclo[12.12.12.13,7.18,12.  
 116,20.121,25.128,32.133,37]tetraconta-3,5,7(44),8,10,12(43),16,18,20  
 (42),21,23,25(41),28(40),29,31,33(39),34,36-octadecaene-  
 κN1,κN14,κN39,κN40,κN41,κN42,κN4  
 3,κN44)-, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



RN 113031-11-1 CAPLUS

CN Europium(3+), (1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene- $\kappa$ N1, $\kappa$ N14, $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42, $\kappa$ N43, $\kappa$ N44)-, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

73

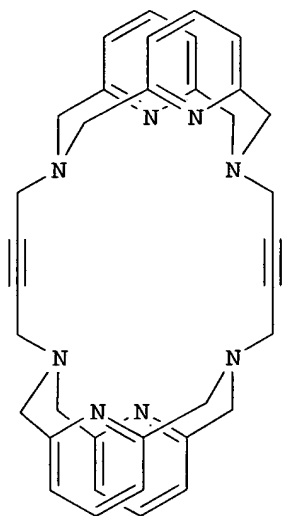
THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 29 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER 2001:540898 CAPLUS

Searched by John DiNatale 571-272-2557

Page 183

DOCUMENT NUMBER: 135:273026  
 TITLE: A Bioinspired Dicopper(II) Catalyst for the  
 Transesterification of Dimethyl **Phosphate**  
 AUTHOR(S): Kuehn, Ulrike; Warzeska, Sabine; Pritzkow, Hans;  
 Kraemer, Roland  
 CORPORATE SOURCE: Anorganisch-Chemisches Institut, Heidelberg, 69120,  
 Germany  
 SOURCE: Journal of the American Chemical Society (2001),  
 123(33), 8125-8126  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:273026  
 GI



I

- AB LCu<sub>2</sub>4<sup>+</sup> (L = I) is the 1st nonenzymic catalyst for the transesterification of simple alkyl, aryl and alkyl/aryl **phosphodiester**s (e.g. O<sub>2</sub>P(OMe)<sub>2</sub>-) under mild conditions. It may operate by a mechanism proposed for hydrolytic or alcoholic **phosphoryl** transfer in various enzymes. The crystal and mol. structures of [LCu<sub>3</sub>(μ<sub>3</sub>-OH)(μ-CH<sub>3</sub>O)<sub>2</sub>(CH<sub>3</sub>CN)<sub>2</sub>](ClO<sub>4</sub>)<sub>3</sub> were determined by x-ray crystallog.
- CC 29-9 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 7, 22, 67, 75, 78
- ST crystal structure copper octaaza macrocycle dinuclear complex; mol structure copper octaaza macrocycle dinuclear complex; copper octaaza macrocycle dinuclear complex catalysis diorganyl **phosphate** transesterification
- IT Transesterification catalysts  
 (copper octaaza-macrocyclic dinuclear complex for diorganyl **phosphates**)
- IT Transesterification kinetics  
 (of diorganyl **phosphates** in presence of copper octaaza-macrocyclic dinuclear complex)
- IT 4043-96-3, Sodium bis(4-nitrophenyl) **phosphate** 32586-82-6, Sodium dimethyl **phosphate** 97174-13-5, Sodium dibenzyl



**phosphate** 363150-87-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(bioinspired dicopper(II) catalyst for transesterification of)

IT **363150-86-1**

RL: CAT (Catalyst use); USES (Uses)

(bioinspired dicopper(II) catalyst for transesterification of diorganyl **phosphates**)

IT 645-15-8, Bis(4-nitrophenyl) **phosphate**

RL: CAT (Catalyst use); USES (Uses)

(inhibition of transesterification of diorganyl **phosphate** monoanion in presence of copper octaaza-macrocyclic dinuclear complex by)

IT **363150-90-7P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

IT **363150-86-1**

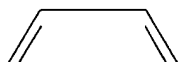
RL: CAT (Catalyst use); USES (Uses)

(bioinspired dicopper(II) catalyst for transesterification of diorganyl **phosphates**)

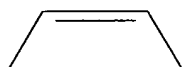
RN 363150-86-1 CAPLUS

CN Copper, tetrakis(nitrato- $\kappa$ O) [ $\mu$ -(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.7.6,14.18,12.121,25.128,32.137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-dodecaene-3,16-diyne- $\kappa$ N1, $\kappa$ N19, $\kappa$ N34, $\kappa$ N35: $\kappa$ N6, $\kappa$ N14, $\kappa$ N43, $\kappa$ N44)]di- (9CI) (CA INDEX NAME)

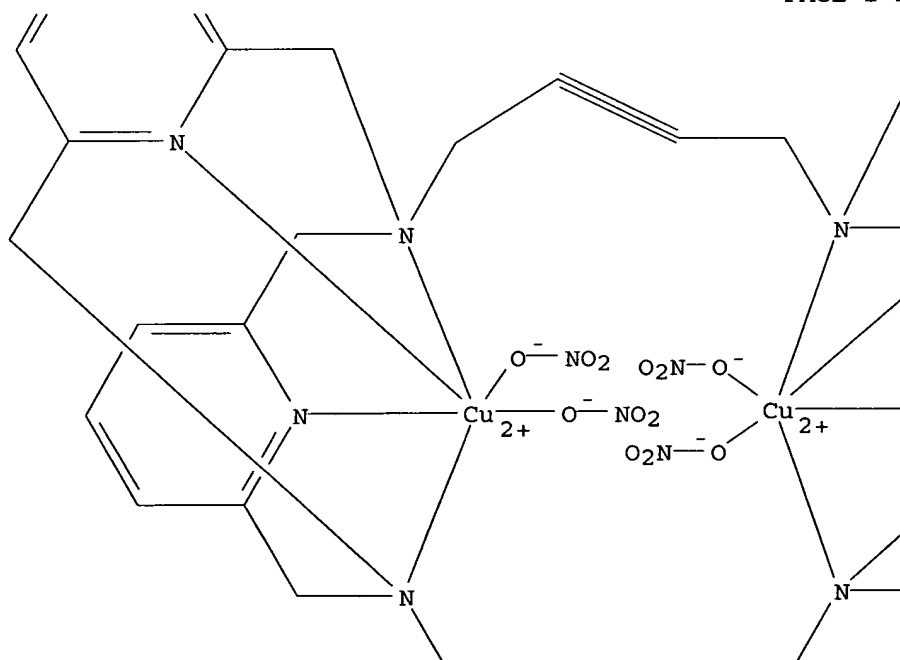
PAGE 1-A



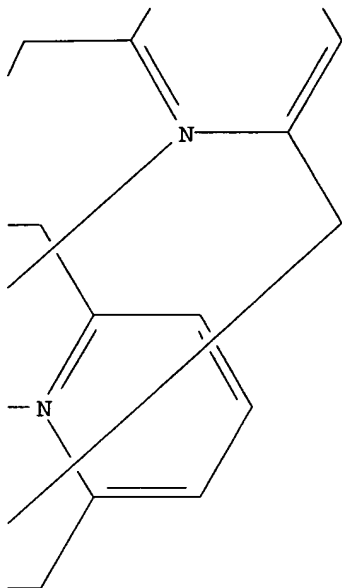
PAGE 1-B



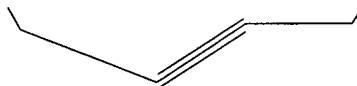
PAGE 2-A



PAGE 2-B



PAGE 3-A

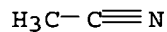


IT **363150-90-7P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 363150-90-7 CAPLUS  
 CN Copper(3+), bis(acetonitrile)-μ<sub>3</sub>-hydroxydi-μ-methoxy[μ-(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.7.6,14.18,12.121,25.128,32.137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-dodecaene-3,16-diyne-κN1,κN19,κN34,κN35:κN6,κN14,κN43,κN44)]tri-, stereoisomer, triperchlorate, compd. with acetonitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



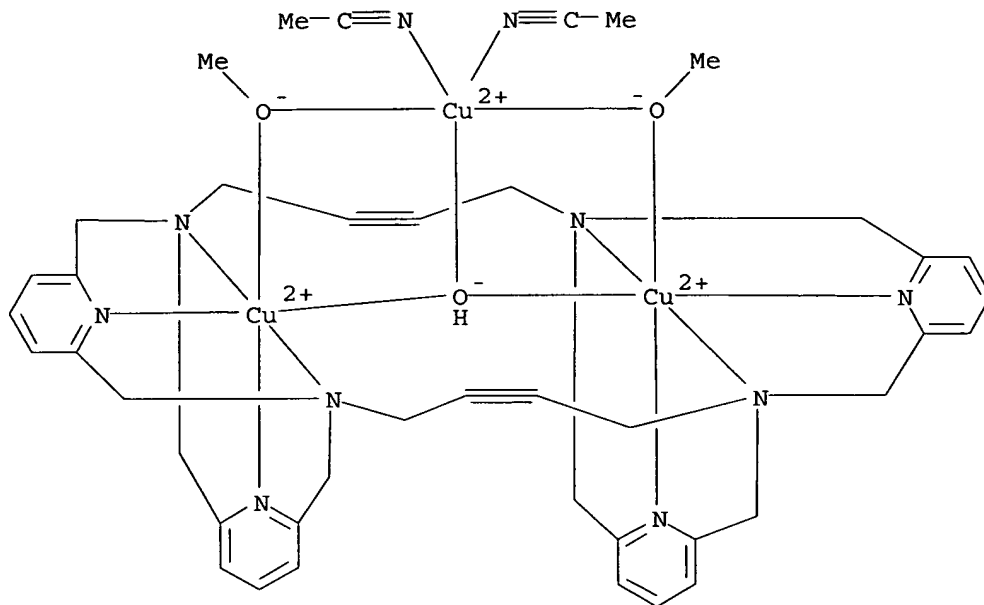
CM 2

CRN 363150-89-4

CMF C42 H49 Cu3 N10 O3 . 3 Cl O4

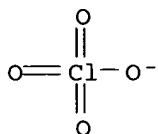
CM 3

CRN 363150-88-3  
 CMF C42 H49 Cu3 N10 O3  
 CCI CCS



CM 4

CRN 14797-73-0  
 CMF Cl O4



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 30 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:530442 CAPLUS

DOCUMENT NUMBER: 135:207684

TITLE: **Fluorescent** Sensors for Zn<sup>2+</sup> Based on a **Fluorescein** Platform: Synthesis, Properties and **Intracellular** Distribution

AUTHOR(S): Burdette, Shawn C.; Walkup, Grant K.; Spingler, Bernhard; Tsien, Roger Y.; Lippard, Stephen J.  
 CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (2001), 123(32), 7831-7841  
 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Two new **fluorescent** sensors for Zn<sup>2+</sup> that utilize **fluorescein** as a reporting group, Zinpyr-1 and Zinpyr-2, have been synthesized and characterized. Zinpyr-1 is prepared in one step via a Mannich reaction, and Zinpyr-2 is obtained in a multistep synthesis that utilizes 4',5'-**fluorescein** dicarboxaldehyde as a key intermediate. Both Zinpyr sensors have excitation and emission wavelengths in the visible range (.apprx.500 nm), dissociation consts. (Kd1) for Zn<sup>2+</sup> of <1 nM, quantum yields approaching unity ( $\Phi$  = .apprx.0.9), and cell permeability, making them well-suited for **intracellular** applications. A 3- to 5-fold **fluorescent** enhancement is observed under simulated physiol. conditions corresponding to the binding of the Zn<sup>2+</sup> cation to the sensor, which inhibits a photoinduced electron transfer (PET) quenching pathway. The x-ray crystal structure of a 2:1 Zn<sup>2+</sup>:Zinpyr-1 complex has also been solved, and is the first structurally characterized example of a complex of **fluorescein** substituted with metal binding ligands.

CC 9-5 (Biochemical Methods)

ST sensor **fluorescent** zinc synthesis

IT Animal cell line  
 (COS-7; reaction with dipicolylamine)

IT Sensors  
 (**fluorescent**; **fluorescent** sensors for Zn<sup>2+</sup> based on **fluorescein** platform-synthesis, properties and **intracellular** distribution)

IT Absorption spectra  
 Crystal structure  
 Fluorescence  
 Fluorescent probes  
 (reaction with dipicolylamine)

IT 7440-66-6, Zinc, analysis  
 RL: ANT (Analyte); ANST (Analytical study)  
 (**fluorescent** sensors for Zn<sup>2+</sup> based on **fluorescein** platform-synthesis, properties and **intracellular** distribution)

IT 288574-78-7P, Zinpyr-1 357916-12-2P, Zinpyr 2  
 RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
 (**fluorescent** sensors for Zn<sup>2+</sup> based on **fluorescein** platform-synthesis, properties and **intracellular** distribution)

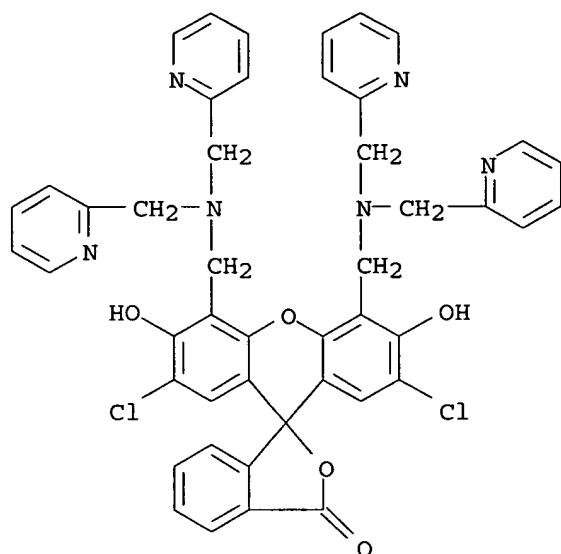
IT 76-54-0, 2',7'-Dichlorofluorescein  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with dipicolylamine)

IT 29227-68-7, Dipicolylamine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with **fluoresceindicarboxaldehyde**)

IT 288574-78-7P, Zinpyr-1 357916-12-2P, Zinpyr 2  
 RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
 (**fluorescent** sensors for Zn<sup>2+</sup> based on **fluorescein** platform-synthesis, properties and **intracellular** distribution)

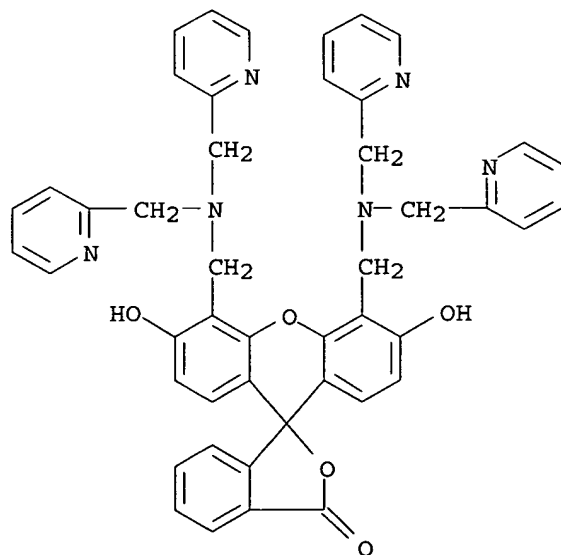
RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



RN 357916-12-2 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9' - [9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 31 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:791144 CAPLUS

DOCUMENT NUMBER: 134:86494

TITLE: Europium cryptate labeled deoxyuridine-triphosphate analog: synthesis and enzymatic incorporation

AUTHOR(S): Alpha-Bazin, B.; Bazin, H.; Guillemer, S.; Sauvaigo,

S.; Mathis, G.  
CORPORATE SOURCE: CIS biointernational/DIVT/Research and New  
technologies, Bagnols/Ceze, F-30 203, Fr.  
SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2000),  
19(9), 1463-1474  
CODEN: NNNAFY; ISSN: 1525-7770  
PUBLISHER: Marcel Dekker, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 134:86494

AB The synthesis of an europium tris-bipyridine cryptate labeled  
2'-deoxyuridine-5'-**triphosphate** analog (K-11-dUTP) is described.  
This labeled **triphosphate** was incorporated into DNA through  
enzymic reactions with terminal transferase and DNA polymerases. The  
enzymic reactions were monitored by TRACE (Time Resolved Amplification of  
Cryptate Emission), a homogeneous method using **Fluorescence**  
Resonance Energy Transfer (FRET) from an europium cryptate as donor to a  
modified allophycocyanine as acceptor.

CC 33-10 (Carbohydrates)  
Section cross-reference(s): 9

ST dUTP europium cryptate labeled prepn polymerase substrate  
**fluorescence**; europium cryptate deoxyuridine **phosphate**  
analog prepn enzymic DNA incorporation

IT Rare earth complexes  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(Europium; synthesis and enzymic incorporation of a europium cryptate  
labeled deoxyuridine-**triphosphate** analog)

IT **Fluorescence**  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

IT **316374-80-8P**  
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN  
(Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC  
(Process)  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

IT 9012-90-2 9027-67-2  
RL: CAT (Catalyst use); USES (Uses)  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

IT 116840-18-7 117032-51-6 **125433-99-0**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

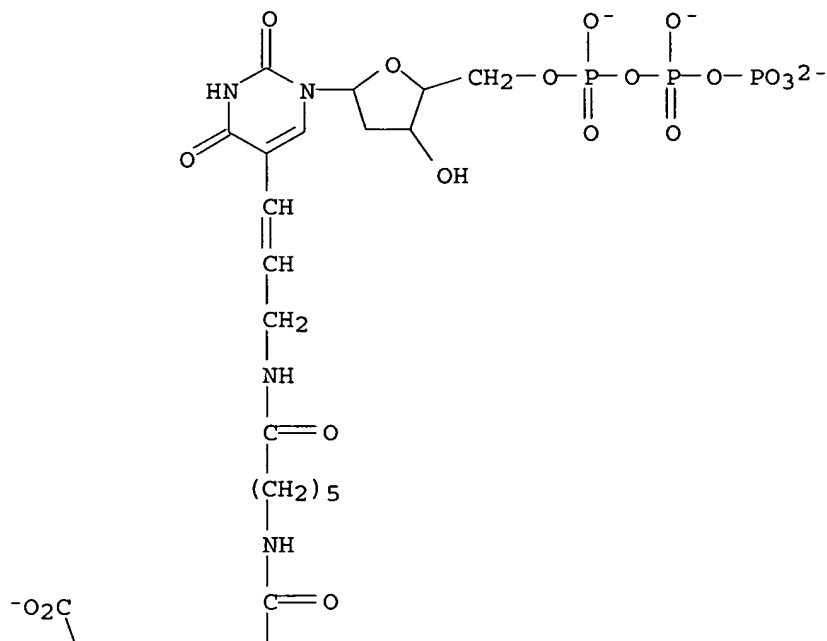
IT **221641-64-1P** 221647-78-5P 316374-81-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

IT **316374-80-8P**  
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN  
(Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC  
(Process)  
(synthesis and enzymic incorporation of a europium cryptate labeled  
deoxyuridine-**triphosphate** analog)

RN 316374-80-8 CAPLUS

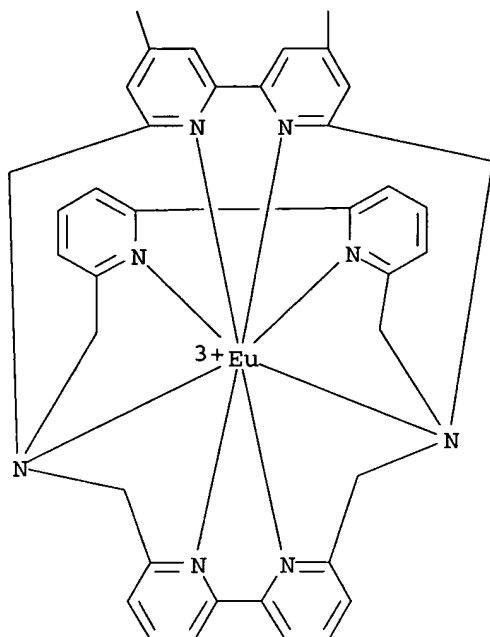
CN Europate(2-), [10-[[[6-[[[(2E)-3-[1-[2-deoxy-5-O-  
[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]- $\beta$ -D-erythro-  
pentofuranosyl]-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl]-2-  
propenyl]amino]-6-oxohexyl]amino]carbonyl]-1,14,39,40,41,42,43,44-

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PAGE 3-A

● 5 H<sup>+</sup>

IT 125433-99-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and enzymic incorporation of a europium cryptate labeled  
 deoxyuridine-triphosphate analog)

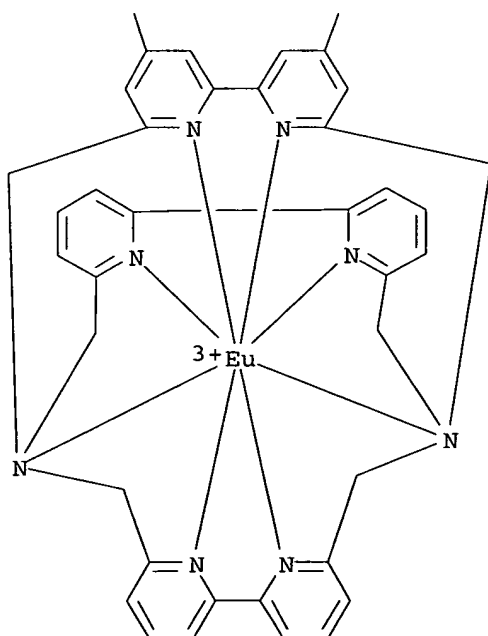
RN 125433-99-0 CAPLUS

CN Europium(3+), (dimethyl 1,14,39,40,41,42,43,44-  
 octaazaocyclotetradecaphenyl[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetr  
 aconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,  
 37(39)-octadecaene-5,10-dicarboxylate-κN1,κN14,κN39,.kap  
 pa.N40,κN41,κN42,κN43,κN44) - (9CI) (CA INDEX  
 NAME)

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IT 221641-64-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

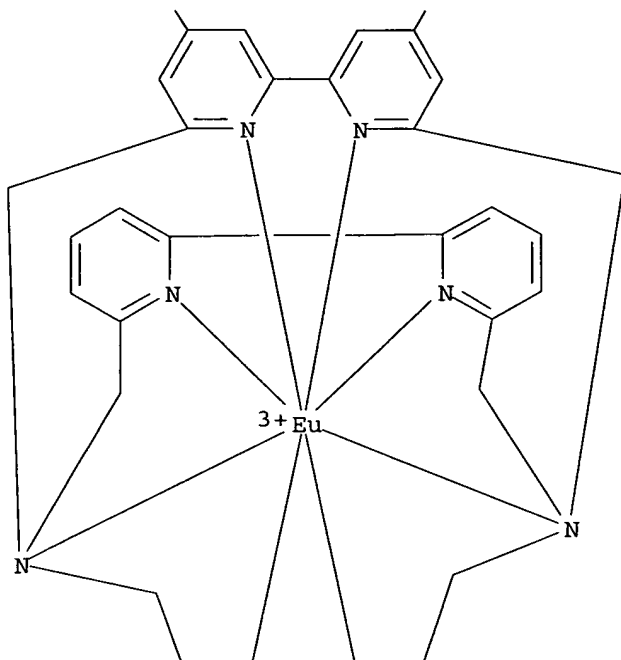
(synthesis and enzymic incorporation of a europium cryptate labeled deoxyuridine-**triphosphate** analog)

RN 221641-64-1 CAPLUS  
CN Europium(1+), [1,14,39,40,41,42,43,44-octaazaocyclotetradeca-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5,10-dicarboxylato(2-)-κN1,κN14,κN39,κN40,κN41,.kappa.N42,κN43,κN44]-, dihydrogen (9CI) (CA INDEX NAME)

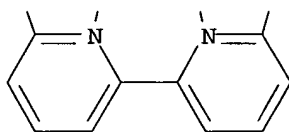
PAGE 1-A



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PAGE 3-A

● 2 H<sup>+</sup>

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 32 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2000:736825 CAPLUS  
 DOCUMENT NUMBER: 134:175180  
 TITLE: Europium Cryptate-Tethered Ribonucleotide for the Labeling of RNA and Its Detection by Time-Resolved Amplification of Cryptate Emission  
 AUTHOR(S): Alpha-Bazin, Beatrice; Bazin, Herve; Boissy, Lilian; Mathis, Gerard  
 CORPORATE SOURCE: Division of In Vitro Technologies, BP 84175, Cis Bio International, Bagnols sur Ceze, F-30204, Fr.  
 SOURCE: Analytical Biochemistry (2000), 286(1), 17-25  
 CODEN: ANBCA2; ISSN: 0003-2697  
 PUBLISHER: Academic Press  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB TRACE (time-resolved amplification of cryptate emission), also called HTRF for pharmaceutical applications, is a homogeneous time-resolved **fluorescence** technique well adapted for the study of mol. interactions. It is based on **fluorescence** resonance energy transfer (FRET) between europium trisbipyridine cryptate (TBPEu3+) as energy donor and cross-linked allophycocyanin, symbolized by XL665, as acceptor, leading to a long-lived FRET signal. TBPEu3+-labeled uridine **triphosphate** (UTP), referred to as K-11-UTP in the text, was obtained by coupling TBPEu3+ moiety to a C-5 functionalized UTP analog. K-11-UTP can be directly incorporated in RNA strands during enzymic synthesis. This was demonstrated in an in vitro transcription reaction promoted by T7 RNA polymerase. The reaction was performed in the presence of K-11-UTP and biotin-labeled cytidine **triphosphate** (biotin-16-CTP) in admixt. with natural ribonucleotides. After the addition of streptavidin-XL665 conjugate (SA-XL665), which binds on biotinylated cytidine residues, a long-lived FRET signal was obtained. This proved that both europium cryptate and biotin were incorporated into the same RNA strand and are close enough to generate a FRET signal. The study of this FRET detection assay format showed that such doubly labeled RNA can be easily detected even when a very low percentage of K-11-UTP is used (less than 1% of total UTP concentration). Europium-cryptate-labeled RNA can also be monitored using a homogeneous hybridization assay format involving a biotinylated probe. After the addition of SA-XL665, the FRET signal generated demonstrates the formation of RNA:DNA hybrids. Europium-cryptate-labeled nucleotide thus gives access to a new type of RNA non-isotopic labeling and homogeneous detection assays. (c) 2000 Academic Press.

CC 9-14 (Biochemical Methods)  
Section cross-reference(s): 3

ST europium cryptate ribonucleotide labeling RNA **fluorescence**  
resonant energy transfer

IT Resonant energy transfer  
(**fluorescence**; europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

IT 221641-67-4D, conjugate with RNA  
RL: ANT (Analyte); ANST (Analytical study)  
(europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

IT 65-47-4D, Cytidine **triphosphate**, biotin labeled  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

IT 221641-67-4P  
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

IT 112131-73-4 221641-64-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

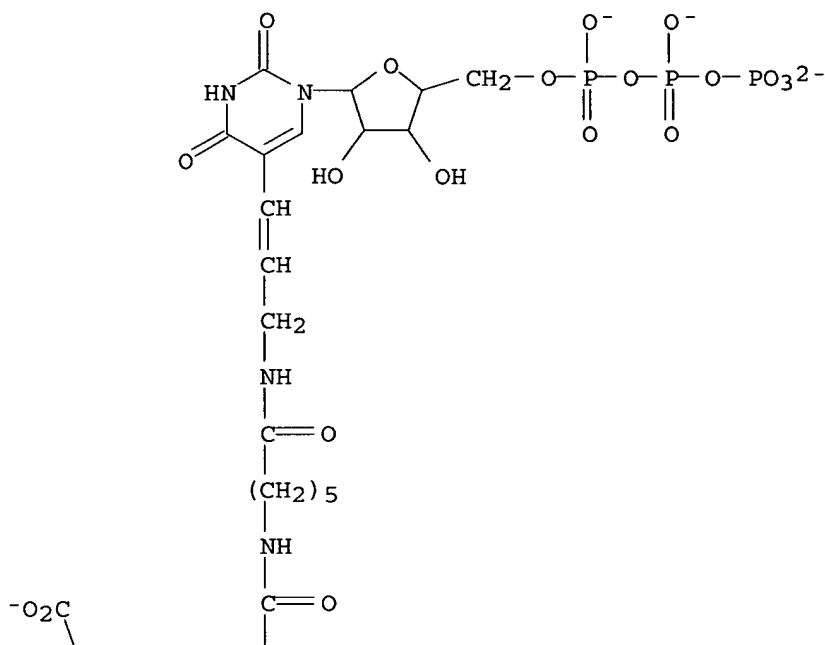
IT 221641-67-4D, conjugate with RNA  
RL: ANT (Analyte); ANST (Analytical study)  
(europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

RN 221641-67-4 CAPLUS

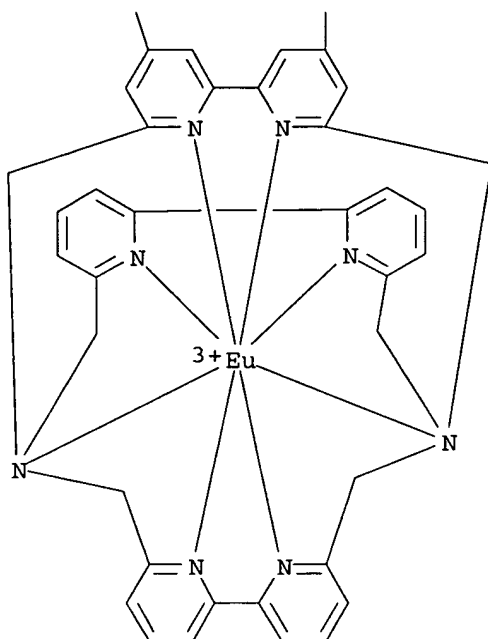
CN Europate(2-), [10-[[[6-oxo-6-[[[(2E)-3-[1,2,3,4-tetrahydro-1-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-

ribofuranosyl]-2,4-dioxo-5-pyrimidinyl]-2-propenyl]amino]hexyl]amino]carbo  
 nyl]-1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.116,20.12  
 1,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,2  
 3,25(41),28,30,32(40),33,35,37(39)-octadecaene-5-carboxylato(5-)-  
 $\kappa$ N1, $\kappa$ N14, $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42, $\kappa$ N4  
 3, $\kappa$ N44]-, monohydrogen (9CI) (CA INDEX NAME)

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PAGE 3-A

● H<sup>+</sup>

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

IT 221641-64-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (europium cryptate-tethered ribonucleotide for labeling of RNA and detection by time-resolved amplification of cryptate emission)

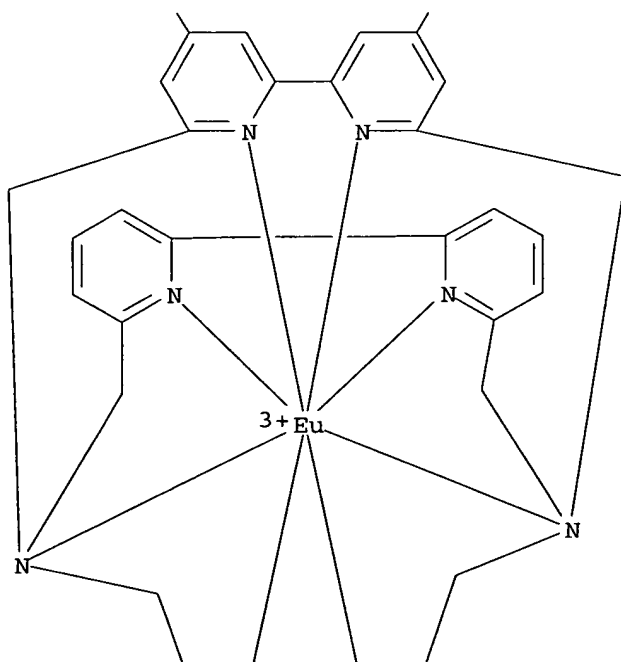
RN 221641-64-1 CAPLUS

CN Europium(1+), [1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5,10-dicarboxylato(2-)-κN1,κN14,κN39,κN40,κN41,.kappa appa.N42,κN43,κN44]-, dihydrogen (9CI) (CA INDEX NAME)

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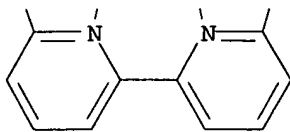


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● 2 H<sup>+</sup>

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 33 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:356015 CAPLUS

DOCUMENT NUMBER: 133:174121

TITLE: ~~A New Cell-Permeable Fluorescent~~  
Probe for Zn<sup>2+</sup>

AUTHOR(S): Walkup, Grant K.; Burdette, Shawn C.; Lippard, Stephen J.; Tsien, Roger Y.

CORPORATE SOURCE: Department of Pharmacology and Chemistry and  
Biochemistry, Howard Hughes Medical Institute  
University of California at San Diego, La Jolla, CA,  
92093-0647, USA

SOURCE: Journal of the American Chemical Society (2000),  
122(23), 5644-5645

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors have prepared a new, high affinity, selective  
**fluorescent** sensor, Zinpyr-1, for zinc that is membrane permeable.  
The **fluorescein** core of Zinpyr-1 exhibits bright  
**fluorescence**, can be excited at visible wavelengths, and overlaps  
well with the 488 nm Ar<sup>+</sup>/ion laser line, which will facilitate confocal  
microscopy with this probe. Zinpyr-1 represents the first Zn<sup>2+</sup> indicator  
to be developed in an ongoing program to tune the binding and optical  
properties of sensors for the neurosciences.

CC 9-4 (Biochemical Methods)  
Section cross-reference(s): 6, 79

ST zinc **fluorescent** probe stain Zinpyr 1 microscopy

IT Animal **cell** line  
(COS-7; new **cell**-permeable **fluorescent** probe for  
Zn<sup>2+</sup>)

IT Staining, biological  
Stains, biological  
(**fluorescent**; new **cell**-permeable  
**fluorescent** probe for Zn<sup>2+</sup>)

IT Complexation  
**Fluorescence** microscopy  
**Fluorescent** probes  
**Fluorometry**  
(new **cell**-permeable **fluorescent** probe for Zn<sup>2+</sup>)

IT 288574-78-7P, Zinpyr 1

RL: ARG (Analytical reagent use); BPR (Biological process); BSU  
(Biological study, unclassified); BUU (Biological use, unclassified); SPN  
(Synthetic preparation); ANST (Analytical study); BIOL (Biological study);

PREP (Preparation); PROC (Process); USES (Uses)

(Zinpyr 1; new **cell-permeable fluorescent** probe for Zn<sup>2+</sup>)

IT 7440-43-9, Cadmium, analysis 7440-66-6, Zinc, analysis 23713-49-7, Zinc(II) ion, analysis

RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(new **cell-permeable fluorescent** probe for Zn<sup>2+</sup>)IT 76-54-0, 2',7'-**Dichlorofluorescein** 1539-42-0 30525-89-4, Paraformaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

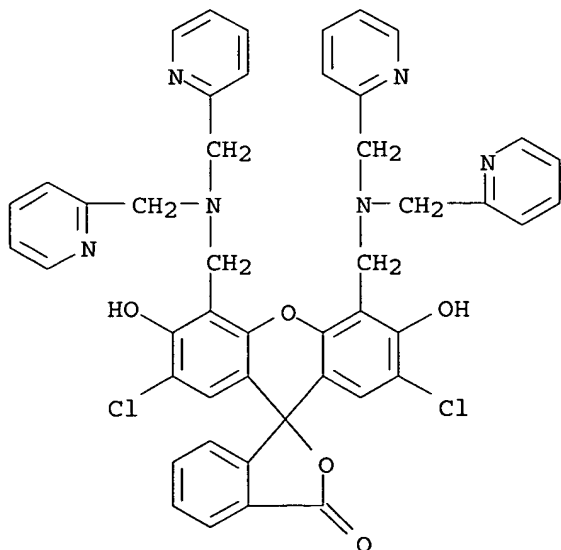
(new **cell-permeable fluorescent** probe for Zn<sup>2+</sup>)IT **288574-78-7P**, Zinpyr 1

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(Zinpyr 1; new **cell-permeable fluorescent** probe for Zn<sup>2+</sup>)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 34 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:161523 CAPLUS

DOCUMENT NUMBER: 132:209505

TITLE:

Bleaching fabrics by atmospheric oxygen in the presence of transition metal complex catalysts  
Appel, Adrianus Cornelis Maria; Carina, Riccardo Filippo; Delroisse, Michel Gilbert Jose; Feringa, Bernard Lucas; Girerd, Jean-jacques; Hage, Ronald; Kalmeijer, Robertus Everardus; Martens, Constantinus

INVENTOR(S):

Franciscus; Peelen, Jacobus Carolina Johannes; Que,  
Lawrence; Swarthoff, Ton; Tetard, David; Thornthwaite,  
David; Tiwari, Laxmikant; Thijssen, Rob; Twisker,  
Robin Stefan; Veerman, Simon Marinus; Van Der Voet,  
Gerrit; Smith, Richard George

PATENT ASSIGNEE(S): Unilever Plc, UK; Unilever Nv; Hindustan Lever Limited  
SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 13  
PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO.   | DATE     |
|---|------|----------|-------------------|----------|
| WO 2000012808   | A1   | 20000309 | WO 1999-GB2878    | 19990901 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW                 |      |          |                   |          |
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| CA 2342616  | AA   | 20000309 | CA 1999-2342616   | 19990901 |
| AU 9956370  | A1   | 20000321 | AU 1999-56370     | 19990901 |
| US 6245115  | B1   | 20010612 | US 1999-388171    | 19990901 |
| EP 1109965  | A1   | 20010627 | EP 1999-943085    | 19990901 |
| EP 1109965  | B1   | 20050601 |                   |          |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO   |      |          |                   |          |
| TR 200101257  | T2   | 20010821 | TR 2001-200101257 | 19990901 |
| BR 9913367  | A    | 20020129 | BR 1999-13367     | 19990901 |
| EP 1433840  | A1   | 20040630 | EP 2004-7615      | 19990901 |
| R: BE, DE, ES, FR, GB, IT   |      |          |                   |          |
| RU 2240391  | C2   | 20041120 | RU 2001-108575    | 19990901 |
| AT 296915   | E    | 20050615 | AT 1999-943085    | 19990901 |
| ES 2243071  | T3   | 20051116 | ES 1999-943085    | 19990901 |
| CA 2364605  | AA   | 20001012 | CA 2000-2364605   | 20000322 |
| WO 2000060043   | A1   | 20001012 | WO 2000-EP2587    | 20000322 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW |      |          |                   |          |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  |      |          |                   |          |
| WO 2000060044   | A1   | 20001012 | WO 2000-EP2590    | 20000322 |
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| TR 200102775  | T2   | 20011221 | TR 2001-200102775 | 20000322 |
| EP 1165738  | A1   | 20020102 | EP 2000-918830    | 20000322 |
| EP 1165738  | B1   | 20050727 |                   |          |

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IE, SI, LT, LV, FI, RO

BR 2000009457 A 20020108 BR 2000-9457 20000322  
AT 300604 E 20050815 AT 2000-918830 20000322  
ES 2244424 T3 20051216 ES 2000-918830 20000322  
US 6617299 B1 20030909 US 2000-539756 20000331  
CA 2382114 AA 20010308 CA 2000-2382114 20000804  
CA 2382115 AA 20010308 CA 2000-2382115 20000804  
WO 2001016268 A1 20010308 WO 2000-EP7561 20000804

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WO 2001016269 A1 20010308 WO 2000-EP7563 20000804

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BR 2000013592 A 20020507 BR 2000-13592 20000804  
BR 2000013593 A 20020507 BR 2000-13593 20000804  
EP 1208184 A1 20020529 EP 2000-951477 20000804

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EP 1208187 A1 20020529 EP 2000-960390 20000804

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TR 200200535 T2 20020722 TR 2002-200200535 20000804  
AU 777434 B2 20041014 AU 2000-64400 20000804  
CA 2383590 AA 20010308 CA 2000-2383590 20000816  
CA 2383596 AA 20010308 CA 2000-2383596 20000816  
CA 2383935 AA 20010308 CA 2000-2383935 20000816  
WO 2001016270 A1 20010308 WO 2000-EP8075 20000816

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WO 2001016271 A1 20010308 WO 2000-EP8076 20000816

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ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
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| WO 2001016261   | A2 | 20010308 | WO 2000-EP8078 20000816    |
| WO 2001016261   | A3 | 20010830 |                            |
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| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  |    |          |                            |
| BR 2000013746   | A  | 20020507 | BR 2000-13746 20000816     |
| BR 2000013744   | A  | 20020514 | BR 2000-13744 20000816     |
| EP 1208185  | A2 | 20020529 | EP 2000-953179 20000816    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL   |    |          |                            |
| EP 1208186  | A1 | 20020529 | EP 2000-958470 20000816    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL   |    |          |                            |
| EP 1208188  | A1 | 20020529 | EP 2000-962335 20000816    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL   |    |          |                            |
| BR 2000013737   | A  | 20020604 | BR 2000-13737 20000816     |
| TR 200201129  | T2 | 20020722 | TR 2002-200201129 20000816 |
| TR 200201130  | T2 | 20020821 | TR 2002-200201130 20000816 |
| TR 200201131  | T2 | 20020923 | TR 2002-200201131 20000816 |
| AU 757351   | B2 | 20030220 | AU 2000-69973 20000816     |
| US 6302921  | B1 | 20011016 | US 2000-649668 20000829    |
| US 6451752  | B1 | 20020917 | US 2000-650139 20000829    |
| ZA 2001001671   | A  | 20020228 | ZA 2001-1671 20010228      |
| ZA 2001001672   | A  | 20020228 | ZA 2001-1672 20010228      |
| ZA 2002000933   | A  | 20030203 | ZA 2002-933 20020201       |
| ZA 2002000934   | A  | 20030203 | ZA 2002-934 20020201       |
| US 2003045442   | A1 | 20030306 | US 2002-112992 20020401    |
| US 6653271  | B2 | 20031125 |                            |

PRIORITY APPLN. INFO.:

|                |    |          |
|----------------|----|----------|
| GB 1998-19046  | A  | 19980901 |
| GB 1999-6474   | A  | 19990319 |
| GB 1999-7713   | A  | 19990401 |
| GB 1999-7714   | A  | 19990401 |
| EP 1999-943083 | A3 | 19990901 |
| WO 1999-GB2876 | A  | 19990901 |
| WO 1999-GB2878 | W  | 19990901 |
| GB 2000-4844   | A  | 20000229 |
| GB 2000-4847   | A  | 20000229 |
| GB 2000-4849   | A  | 20000229 |
| GB 2000-4850   | A  | 20000229 |
| GB 2000-4858   | A  | 20000229 |
| GB 2000-4990   | A  | 20000301 |
| GB 2000-6961   | A  | 20000322 |
| WO 2000-EP2590 | W  | 20000322 |
| WO 2000-EP7561 | W  | 20000804 |
| WO 2000-EP7563 | W  | 20000804 |
| WO 2000-EP8075 | W  | 20000816 |
| WO 2000-EP8076 | W  | 20000816 |
| WO 2000-EP8078 | W  | 20000816 |
| US 2000-650134 | A3 | 20000829 |

OTHER SOURCE(S): MARPAT 132:209505

AB Fabrics such as laundered fabrics are bleached by atmospheric O by treatment with

transition metal complexes, that are applied in the dry form or in aqueous solns. (such as in laundering) or in nonaq. solns. (such in dry cleaning). The method can confer cleaning benefits to the textile after the treatment. A typical complex was manufactured by reaction of 2-pyridyl ketone oxime 1 h in EtOH-NH<sub>4</sub>OH containing NH<sub>4</sub>OAc with Zn at reflux, reaction of the resulting bis(pyridin-2-yl)methylamine 40 h with picolyl chloride hydrochloride in aqueous NaOH, reduction of the perchlorate salt of the 2nd intermediate with LiAlH<sub>4</sub>, lithiation of the 3rd intermediate with BuLi, methylation of 4th intermediate with MeI, and complexation of the resulting ligand with Fe(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O.

IC ICM D06L003-02

CC 46-5 (Surface Active Agents and Detergents)

Section cross-reference(s): 78

IT 16941-11-0, Ammonium **hexafluorophosphate** 21324-39-0, Sodium **hexafluorophosphate**

RL: RCT (Reactant); RACT (Reactant or reagent)

(complex precursor; compns. containing transition metal complex catalysts for bleaching laundered fabrics with atmospheric oxygen)

IT 7439-96-5D, Manganese, bis(pyridinylmethyl)dimethylethylenediamine complex, uses 61920-87-4 **108114-13-2** 116633-52-4

129766-11-6 129766-12-7 133523-08-7 136074-05-0 136768-57-5D, manganese complex 157966-71-7 167695-89-8 260395-40-2 260395-42-4 260395-44-6 260416-70-4 260416-73-7

RL: CAT (Catalyst use); USES (Uses)

(compns. containing transition metal complex catalysts for bleaching laundered fabrics with atmospheric oxygen)

IT **108114-13-2**

RL: CAT (Catalyst use); USES (Uses)

(compns. containing transition metal complex catalysts for bleaching laundered fabrics with atmospheric oxygen)

RN 108114-13-2 CAPLUS

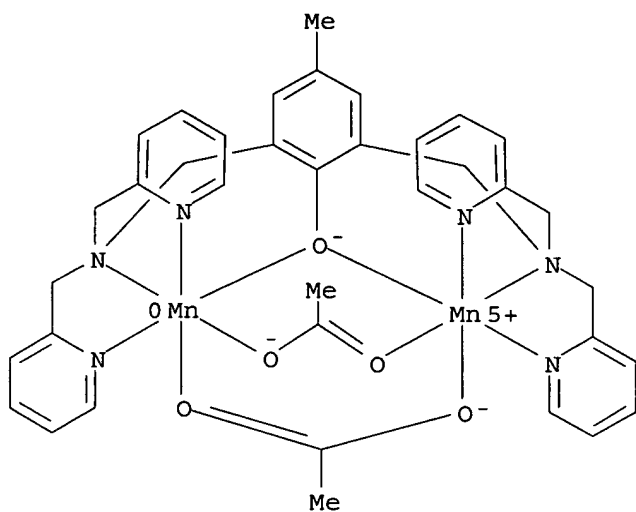
CN Manganese(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-methylphenolato-κO:κO]]di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 108114-12-1

CMF C37 H39 Mn2 N6 O5

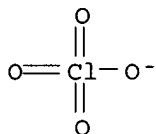
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl 04



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 35 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:673763 CAPLUS

DOCUMENT NUMBER: 132:35884

TITLE: Selective oxidation of [RhI(cod)]<sup>+</sup> by H<sub>2</sub>O<sub>2</sub> and O<sub>2</sub>  
 AUTHOR(S): De Bruin, Bas; Brands, Johanna A.; Donners, Jack J. J. M.; Donners, Maurice P. J.; De Gelder, Rene; Smits, Jan M. M.; Gal, Anton W.; Spek, Anton L.

CORPORATE SOURCE: Department of Inorganic Chemistry, University of Nijmegen, Nijmegen, 6525 ED, Neth.

SOURCE: Chemistry--A European Journal (1999), 5(10), 2921-2936  
 CODEN: CEUJED; ISSN: 0947-6539

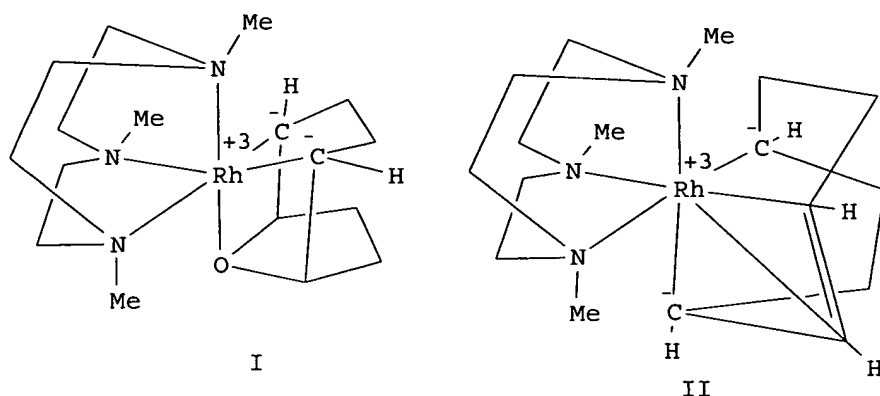
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:35884

GI



AB New, five-coordinate Z,Z-1,5-cyclooctadiene (cod) complexes  $[\text{'N3'}\text{RhI}(\text{cod})]^+$  were structurally characterized by NMR spectroscopy and x-ray diffraction ('N3' = tridentate cyclic triamine or podal pyridine-amine-pyridine ligand). Their electrochem. oxidation and their oxygenation by  $\text{H}_2\text{O}_2$  and  $\text{O}_2$  were studied. The  $\sigma$ -donor capacity of ligand 'N3' in  $[\text{'N3'}\text{RhI}(\text{cod})]^+$  strongly influences the electrochem. oxidation potential and the  $^{13}\text{C}$  chemical shift of the cod double bond. The relative  $\sigma$ -donor strength of the individual amine (NamineR) and pyridine (NPY) nitrogens in the pyridine-amine-pyridine ligands, NamineH > NPY > NPY-Me > NamineBu NamineBz, is largely determined by steric repulsions. The cod complexes are selectively oxygenated by  $\text{H}_2\text{O}_2$ , and in one case by  $\text{O}_2$ , to Rh(III)oxabicyclononanediyl complexes (e.g. I) which rearrange to Rh(III)-hydroxycyclooctenediyl (e.g. II) complexes. Oxygenation of cod to an oxabicyclononanediyl fragment and subsequent rearrangement to a hydroxycyclooctenediyl fragment are both thought to proceed via a 2-rhodaoxetane intermediate. Oxygenation of  $[\text{'N3'}\text{RhI}(\text{cod})]^+$  by  $\text{H}_2\text{O}_2$  is relatively independent of the ligand and the solvent, and proceeds instantaneously and selectively. Oxygenation of  $[\text{'N3'}\text{RhI}(\text{cod})]^+$  by  $\text{O}_2$  is greatly influenced by both the ligand and the solvent. Entirely selective oxidation by  $\text{O}_2$  could only be obtained for 'N3' = N,N-di(2-pyridylmethyl)amine (BPA) in  $\text{CH}_2\text{Cl}_2$ . Oxygenation by  $\text{O}_2$  in  $\text{CH}_2\text{Cl}_2$  requires one mole of  $\text{O}_2$  per mol of  $[(\text{BPA})\text{RhI}(\text{cod})]^+$ , is catalyzed by acid and is likely to proceed by mononuclear activation of dioxygen. For both the cyclic triamine ligands and the podal pyridine-amine-pyridine ligands, the cod complexes with the lowest oxidation potentials are the most reactive and the most selective in oxygenation by  $\text{O}_2$ . Oxidation of the analogous 1,5-hexadiene (hed) complexes  $[\text{'N3'}\text{RhI}(\text{hed})]^+$  by either  $\text{H}_2\text{O}_2$  or  $\text{O}_2$  results in elimination of hed.

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 72, 75

IT 1539-42-0, Bis((2-pyridinyl)methyl)amine 3731-51-9, 2-(Aminomethyl)pyridine 4730-54-5, 1,4,7-Triazacyclononane 26082-96-2, Benzylbis((2-pyridinyl)methyl)amine 96556-05-7, 1,4,7-Trimethyl-1,4,7-triazacyclononane 162339-92-6, 1,4-Bis(bis((2-pyridinyl)methyl)amino)butane

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with rhodium diene chloro dinuclear complex)

IT 252328-22-6P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, crystal structure, fluxionality, electrochem. oxidation and



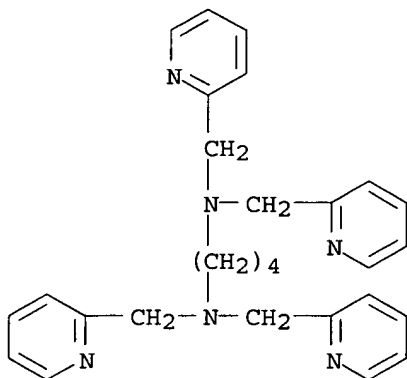
reaction with hydrogen peroxide)

IT 90478-92-5P, (2-(Aminomethyl)pyridine-N,N') (η4-1,5-cyclooctadiene)rhodium(1+) **hexafluorophosphate**  
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation, fluxionality and electrochem. oxidation of)

IT 162339-92-6, 1,4-Bis(bis((2-pyridinyl)methyl)amino)butane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coordinative substitution with rhodium diene chloro dinuclear complex)

RN 162339-92-6 CAPLUS

CN 1,4-Butanediamine, N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



IT 252328-22-6P  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation, crystal structure, fluxionality, electrochem. oxidation and reaction with hydrogen peroxide)

RN 252328-22-6 CAPLUS

CN Rhodium(2+), bis[(1,2,5,6-η)-1,5-cyclooctadiene] [μ-[N,N,N',N'-tetrakis[(2-pyridinyl-κN)methyl]-1,4-butanediamine-κN:κN']]di-, stereoisomer, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

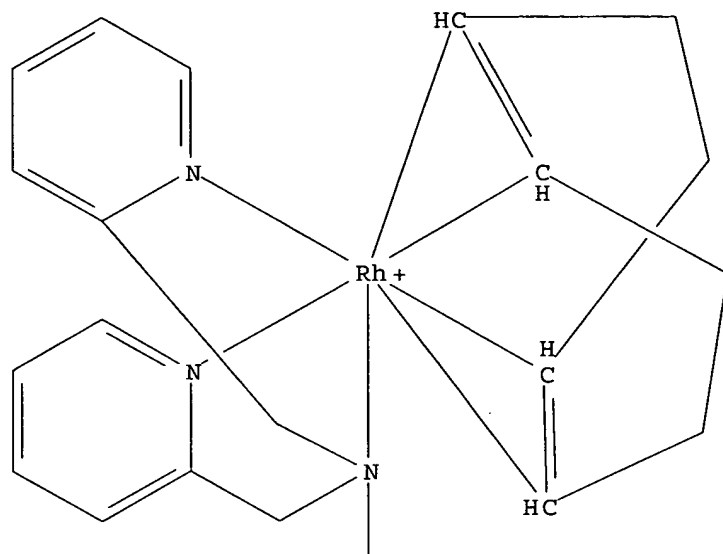
CM 1

CRN 252328-21-5

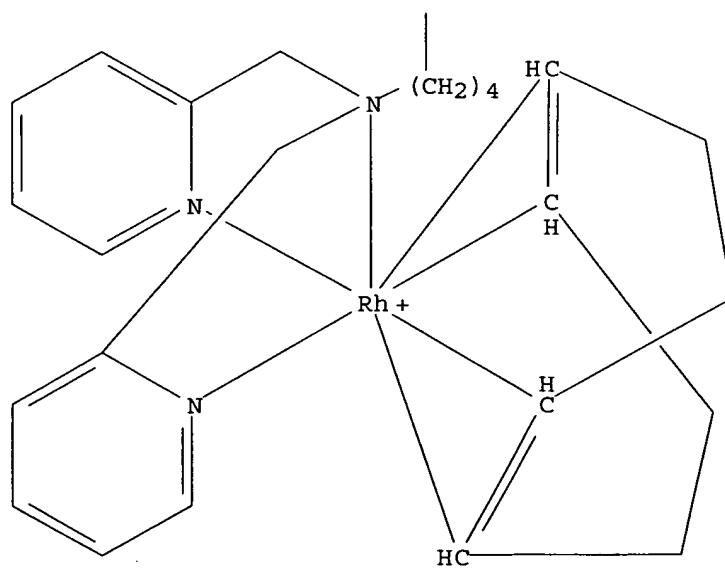
CMF C44 H56 N6 Rh2

CCI CCS

PAGE 1-A



PAGE 2-A

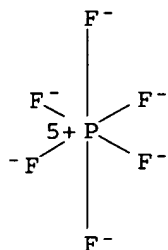


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 36 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:606991 CAPLUS

DOCUMENT NUMBER: 131:225488

TITLE: **Fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance

INVENTOR(S): Tsien, Roger Y.; Zlokarnik, Gregor

PATENT ASSIGNEE(S): The Regents of the University of California, USA

SOURCE: U.S., 58 pp., Cont. of U. S. Ser. No. 727,616.

CODEN: USXXAM

DOCUMENT TYPE: Patent

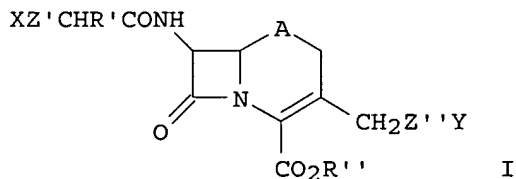
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE        |
|------------------------|------|----------|-----------------|-------------|
| US 5955604             | A    | 19990921 | US 1997-955401  | 19971021    |
| US 6291162             | B1   | 20010918 | US 1996-727616  | 19961015    |
| PRIORITY APPLN. INFO.: |      |          | US 1996-727616  | A1 19961015 |
|                        |      |          | US 1996-732178  | A1 19961016 |
|                        |      |          | US 1995-407544  | A2 19950320 |
|                        |      |          | WO 1996-US4059  | W 19960320  |

OTHER SOURCE(S): MARPAT 131:225488  
GI



AB Substrates for  $\beta$ -lactamase are provided of the general formula I in which one of X and Y is a **fluorescent** donor moiety and the other is a quencher (which may or may not re-emit); R' is selected from the group consisting of H, lower (i.e., alkyl of 1 to about 5 carbon atoms) and (CH<sub>2</sub>)<sub>n</sub>OH, in which n is 0 or an integer from 1 to 5; R'' is selected from the group consisting of H, physiologically acceptable metal and ammonium

cations, -CHR2OCO(CH<sub>2</sub>)<sub>n</sub>CH<sub>3</sub>, -CHR2OCOC(CH<sub>3</sub>)<sub>3</sub>, acylthiomethyl, acyloxy- $\alpha$ -benzyl,  $\delta$ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulfinylmethyl,  $\beta$ -morpholinoethyl, dialkylaminoethyl, acyloxyalkyl, dialkylaminocarbonyloxymethyl and aliphatic, in which R<sub>2</sub> is selected from the group consisting of H and lower alkyl; A is selected from the group consisting of S, O, SO, SO<sub>2</sub> and CH<sub>2</sub>; and Z' and Z'' are linkers for the **fluorescent** donor and quencher moieties. Methods of assaying  $\beta$ -lactamase activity and monitoring expression in systems using  $\beta$ -lactamase as a reporter gene also are disclosed. Examples include Drosophila or zebrafish embryo transformation assays as well as animal **cell** glucocorticoid receptor-mediated or  $\beta$ -adrenergic receptor-mediated transcription assays.

- IC ICM C07D501-14  
ICS C12Q001-34
- INCL 540222000
- CC 7-3 (Enzymes)  
Section cross-reference(s): 1, 3, 10, 26
- ST lactam beta **fluorescent** prepn transcription assay; cephalosporin **fluorogenic** prepn gene transcription assay; lactamase beta reporter gene assay **fluorescence**; transformation genetic assay **fluorescent** beta lactam; antibiotic beta lactam resistance assay **fluorescence**; Bacillus beta lactamase gene sequence Escherichia
- IT Genetic element  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(GRE (glucocorticosteroid-responsive element); **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(RNA formation factor NFAT-1-responsive element; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Gene  
(expression,  $\beta$ -lactamase reporter gene expression; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT **Fluorescence** quenching  
**Fluorescent** probes  
(**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Glucocorticoid receptors  
Reporter gene  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Antibiotics  
( $\beta$ -lactam; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Bacillus licheniformis  
Escherichia coli  
( $\beta$ -lactamase derivs.; **fluorogenic**  $\beta$ -lactam preparation

and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-82-5P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(CCF1, preparation,  $\beta$ -lactam **fluorogenic** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-52-9P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
(CCF2, preparation and reaction with acetoxymethylbromide,  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-66-5P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(CCF2/ac2AM2, preparation, membrane permeable  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-69-8P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(CCF2/btAMac2, preparation, membrane permeant  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-65-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(CCFlac3, preparation and deacylation; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-62-1P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(FCRE, preparation,  $\beta$ -lactam **fluorogenic** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-59-6P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(FCRX, preparation,  $\beta$ -lactam **fluorogenic** derivative;

**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183870-59-9P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(RCF, preparation,  $\beta$ -lactam **fluorogenic** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183869-58-1P 183869-60-5P 183869-62-7P 183869-64-9P 183869-66-1P,  
Lactamase,  $\beta$ - (*Bacillus licheniformis*)

RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(amino acid sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 957-68-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
(conversion to mercapto-cephalosporanic acid and coupling with rhodol derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 51649-83-3, 5-Aminofluorescein

RL: RCT (Reactant); RACT (Reactant or reagent)  
(conversion to **mercaptofluorescein** or bromination;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 26973-80-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling by nucleophilic displacement reaction with **mercaptofluorescein**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-53-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling by nucleophilic displacement with diacetyl eosinithiol;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 120718-52-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction with amine of bifunctional cephalosporin;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 56040-80-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction with coumarin or **fluorescein** derivs.;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-68-7

RL: RCT (Reactant); RACT (Reactant or reagent)

- (coupling reaction with **fluorescein**-cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 125440-93-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling reaction with mercapto-cephalosporin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 68169-37-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling reaction with thiol of bifunctional cephalosporin; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 84461-60-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (displacement reaction with cephalosporin amine bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 11111-12-9D, Cephalosporin, **fluorogenic** derivs.  
 RL: ARG (Analytical reagent use); ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 81-88-9D, cephalosporin **fluorogenic** derivs. 91-64-5D, Coumarin, cephalosporin **fluorogenic** derivs. 93-35-6D, 7-Hydroxycoumarin, cephalosporin **fluorogenic** derivs. 574-93-6D, Phthalocyanine, **fluorogenic**  $\beta$ -lactam derivs. 2320-96-9D, **Dichlorofluorescein**, cephalosporin **fluorogenic** derivs. 2321-07-5D, **Fluorescein**, cephalosporin **fluorogenic** derivs. 3086-44-0D, Rhodol, cephalosporin **fluorogenic** derivs. 7440-27-9D, Terbium, **fluorogenic**  $\beta$ -lactam derivs., biological studies 7440-53-1D, Europium, **fluorogenic**  $\beta$ -lactam derivs., biological studies 17372-87-1D, Eosin, cephalosporin **fluorogenic** derivs. 26761-84-2D, **Tetrachlorofluorescein**, cephalosporin **fluorogenic** derivs. 87893-58-1D, 6-Chloro-7-hydroxycoumarin, cephalosporin **fluorogenic** derivs. 183736-85-8 183736-86-9 183736-87-0  
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 9073-60-3P,  $\beta$ -Lactamase  
 RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription,

- transfection, or antibiotic resistance)
- IT 183869-57-0 183869-59-2 183869-61-6 183869-63-8 183869-65-0  
 RL: ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
 (nucleotide sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-58-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and bromide displacement reaction with **fluoresceinthiol**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-81-4P 183736-83-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cleavage reaction; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-60-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and conversion to eosinthiol diacetate dimer; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 75900-75-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and conversion to mercapto-eosin; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-54-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and coupling by nucleophilic displacement with cephalosporin acetate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-49-4P 183736-56-3DP, bromoacetamide derivs. 183736-78-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and coupling reaction with cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183743-61-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and coupling reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-51-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)



- (preparation and coupling reaction with coumarin-cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-63-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with **fluoresceinthiol** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-80-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with mercapto-**fluorescein** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 56654-74-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reactions with **fluorescein**, rhodamine, or resorufin derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-61-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling with **fluoresceinthiol**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-79-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and conversion to iodo-derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-64-3P 183736-75-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deprotection; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-47-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with benzylglycine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-57-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromoacetyl bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-73-4P

- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromoacetyl bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-84-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromomethylacetate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-74-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with butyric anhydride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 5269-39-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 131088-02-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with malonate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-71-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with resorcinol; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 97461-45-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with silyl-sarcosine derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-76-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction to monomer; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-70-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction to monomers; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-55-2P

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation,  $\beta$ -lactam **fluorescent** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 107-97-1, Sarcosine

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with N-Me **trimethylsilyltrifluoroacetamide**;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 106-31-0, Butyric anhydride 1738-76-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 140-89-6, Potassium ethylxanthate

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with eosinamine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 79349-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with **fluorescein** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 5466-84-2, 4-Nitrophthalic anhydride

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with hydroxyjulolidine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 108-46-3, 1,3-Benzenediol, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with hydroxyjulolidine derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 41175-50-2, 8-Hydroxyjulolidine

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with nitrophthalic anhydride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 24589-78-4, N-Methyl-N-(trimethylsilyl)**trifluoroacetamide**

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with sarcosine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-77-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with thionyl chloride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

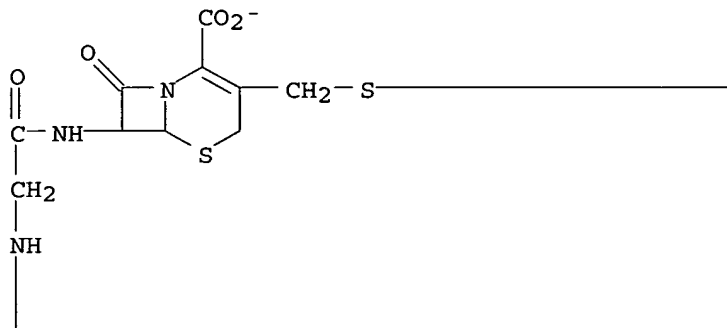
IT 95-88-5, 4-Chlororesorcinol

RL: RCT (Reactant); RACT (Reactant or reagent)

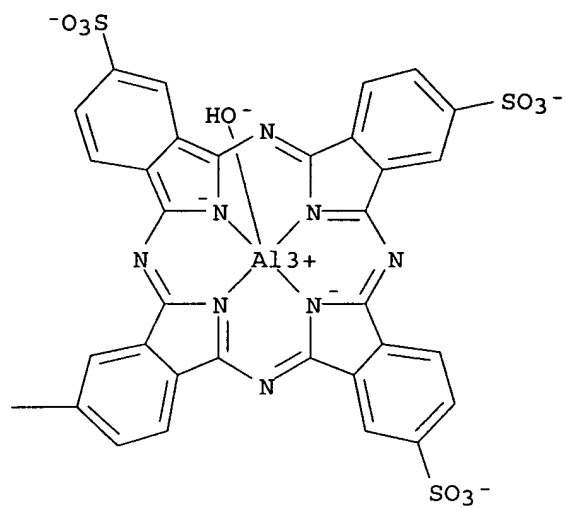
(reaction; **fluorogenic**  $\beta$ -lactam preparation and

$\beta$ -lactamase reporter gene assay for animal **cell**  
 transcription, transfection, or antibiotic resistance)  
 IT 183736-72-3P  
 RL: BYP (Byproduct); PREP (Preparation)  
 (synthetic byproduct; **fluorogenic**  $\beta$ -lactam preparation and  
 $\beta$ -lactamase reporter gene assay for animal **cell**  
 transcription, transfection, or antibiotic resistance)  
 IT 183736-87-0  
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU  
 (Biological study, unclassified); BUU (Biological use, unclassified); PRP  
 (Properties); ANST (Analytical study); BIOL (Biological study); PROC  
 (Process); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase  
 reporter gene assay for animal **cell** transcription,  
 transfection, or antibiotic resistance)  
 RN 183736-87-0 CAPLUS  
 CN Europate(2-), [ $\mu$ -[10-[[[2-[2-carboxy-8-oxo-3-[[[9,16,23-trisulfo-  
 29H,31H-phthalocyanin-2-yl]thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-en-  
 7-yl]amino]-2-oxoethyl]amino]carbonyl]-1,14,39,40,41,42,43,44-  
 octaazaoctacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetr  
 aconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,  
 37(39)-octadecaene-5-carboxylato(8-)-N1,N14,N39,N40,N41,N42,N43,N44:N29,N3  
 0,N31,N32]](hydroxyaluminate)-(9CI) (CA INDEX NAME)

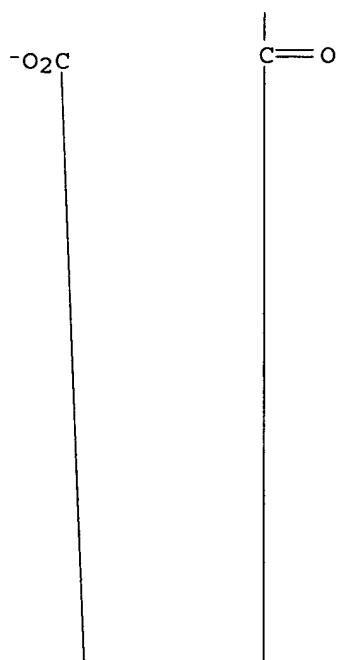
PAGE 1-A



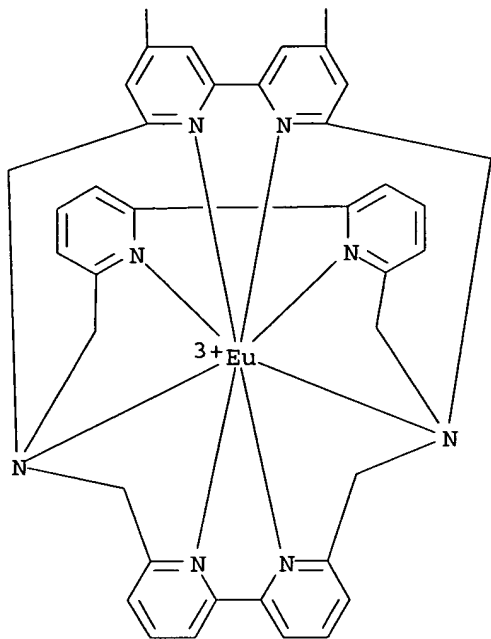
PAGE 1-B



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 37 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:496159 CAPLUS

DOCUMENT NUMBER: 131:294704

TITLE: Synthesis and characterization of dinuclear complexes containing the FeIII-F . . . (H<sub>2</sub>O)MII motif

AUTHOR(S): Ghiladi, Morten; Jensen, Kenneth B.; Jiang, Jianzhong; McKenzie, Christine J.; Morup, Steen; Sotofte, Inger; Ulstrup, Jens

CORPORATE SOURCE: University of Southern Denmark, Main campus, Department of Chemistry, Odense University, Odense, DK-5230, Den.

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (16), 2675-2681  
CODEN: JCOTBI; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dinucleating phenolate-hinged ligand 4-tert-butyl-2,6-bis[bis(2-pyridylmethyl)aminomethyl]phenolate (bpbp-) was used to prepare FeIIIMII complexes containing independent species at the exogenous binding sites. These sites are occupied by fluoride and H<sub>2</sub>O ligands and show the general formulation [(bpbp)Fe(F)2M(H<sub>2</sub>O)<sub>n</sub>][BF<sub>4</sub>]<sub>2</sub>, M = Zn or Cu, n = 1; M = Co or Fe, n = 2. Two terminal F- ions are bound to the Fe(III) ion and one or two H<sub>2</sub>O ligands to the adjacent divalent metal ion. The fluoride ligands are derived from the hydrolysis of tetrafluoroborate. In the crystal structure of [(bpbp)Fe(F)2Cu(H<sub>2</sub>O)][BF<sub>4</sub>]<sub>2</sub>·4H<sub>2</sub>O. The Cu(II) and Fe(III) atoms are linked asym. by the phenolic O atom hinge of bpbp- with Cu-Ophenolato 2.270(2) and Fe-Ophenolato 2.041(2) Å with a

Cu...Fe distance of 3.828(1) Å. The two terminal F<sup>-</sup> ions are bound to the Fe atom (Fe-F 1.818(2), 1.902(2) Å) and one of them is strongly H bonded to the H<sub>2</sub>O mol. on the adjacent Cu atom (F-H...O 2.653(4) Å). The metal ions in the aqua **fluoride** complexes [(bpbp)Fe(F)2M(H<sub>2</sub>O)2][BF<sub>4</sub>]<sub>2</sub>, M = Fe or Co, are weakly antiferromagnetically coupled (J = -8 and -10 cm<sup>-1</sup>, resp.) and in [(bpbp)Fe(F)2Cu(H<sub>2</sub>O)][BF<sub>4</sub>]<sub>2</sub> are weakly ferromagnetically coupled (J = 2 cm<sup>-1</sup>). The spectroscopic, electrochem. and magnetic properties of these complexes are compared to those of an analogous series of complexes containing two acetate bridging groups in the exogenous site. Electrochem. results indicate that the Fe(III) ions in the bis-**fluoride** complexes are stabilized by .apprx.300 mV towards reduction compared to the bis-μ-acetate complexes. The crystal structure of one bis-μ-acetate complex, [Fe<sub>2</sub>(bpbp)(CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>][BF<sub>4</sub>]<sub>2</sub>, shows the expected arrangement; the Fe-(II) and -(III) atoms are triply bridged by the phenolic O atom of bpbp- and two μ-acetate groups with FeII-Ophenolato 2.088(4) and FeIII-Ophenolato 1.951(5) Å and an Fe...Fe distance of 3.380(2) Å.

The crystal structure at 120 K indicates that the Fe atoms are valence trapped and in accordance with this Mossbauer measurements between 80 and 200 K show clearly distinguishable Fe-(II) and -(III) components. The Mossbauer spectra of [(bpbp)Fe(F)2Cu(H<sub>2</sub>O)][BF<sub>4</sub>]<sub>2</sub>·4H<sub>2</sub>O are influenced by paramagnetic relaxation effects with relaxation times of the order of 1 ns. The relaxation time increases when a magnetic field is applied. This effect can be explained by a model for cross-relaxation in conjunction with the crystal symmetry of the compound

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 7, 72, 73, 75, 77

ST crystal structure iron heterodinuclear **difluoro**

butylbisbispyridylmethylaminomethylphenolate; structure iron copper zinc butylbisbispyridylmethylaminomethylphenolate **difluoro**; iron

homodinuclear heterodinuclear **difluoro**

butylbisbispyridylmethylaminomethylphenolate prepn; purple acid

**phosphatase** model **difluoroiron**

butylbisbispyridylmethylaminomethylphenolate

IT Enzyme functional sites

(active; iron homo- and heterodinuclear **difluoro**

butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes as models for purple acid **phosphatase**)

IT Transition metal complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(iron homo- and heterodinuclear **difluoro**

butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua; preparation, structure and electrochem. properties as models for active sites of purple acid **phosphatases**)

IT Ferromagnetic exchange

(of iron copper **difluoro** butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complex)

IT Crystal structure

Molecular structure

(of iron heterodinuclear copper and zinc **difluoro**

butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes)

IT Redox potential

(of iron heterodinuclear **difluoro**

butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes)

IT Mossbauer effect

(of iron homo- and heterodinuclear butylbis[bis(pyridylmethyl)aminomethyl]phenol complexes with and without **fluoride**)

IT Antiferromagnetic exchange

Hydrogen bond

(of iron homo- and heterodinuclear **difluoro**

butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes)

IT Hydrolysis  
(of **tetrafluoroborate** in preparation of iron homo- and heterodinuclear **difluoro** butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes)

IT 202129-01-9 202129-05-3 202129-07-5  
246234-27-5  
RL: PRP (Properties)  
(antiferromagnetic coupling of)

IT 246144-00-3 246144-01-4 246144-02-5  
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
(elec. potential of couple containing)

IT 246144-06-9  
RL: PRP (Properties)  
(ferromagnetic coupling of)

IT 202128-99-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for preparation of iron homo- and heterodinuclear **difluoro** phenol derivative aqua complexes as acid **phosphatase** active site models)

IT 9001-77-8, Acid **phosphatase**  
RL: PRP (Properties)  
(preparation of iron homo- and heterodinuclear **difluoro** phenol derivative aqua complexes as active site models for)

IT 246143-99-7P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, crystal structure and Mossbauer effect of)

IT 246143-94-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, crystal structure, electrochem. magnetic properties of iron homo- and heterodinuclear **difluoro** butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes as acid **phosphatase** active site models)

IT 246143-91-9P 246143-97-5P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, electrochem., magnetic and structural properties of iron homo- and heterodinuclear **difluoro** butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes as acid **phosphatase** active site models)

IT 202129-01-9 202129-05-3 202129-07-5  
246234-27-5  
RL: PRP (Properties)  
(antiferromagnetic coupling of)

RN 202129-01-9 CAPLUS

CN Iron(2+), diaqua[μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]]difluorodi-, stereoisomer, bis[tetrafluoroborate(1-)], tetrahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 246144-03-6

CMF C36 H43 F2 Fe2 N6 O3 . 2 B F4

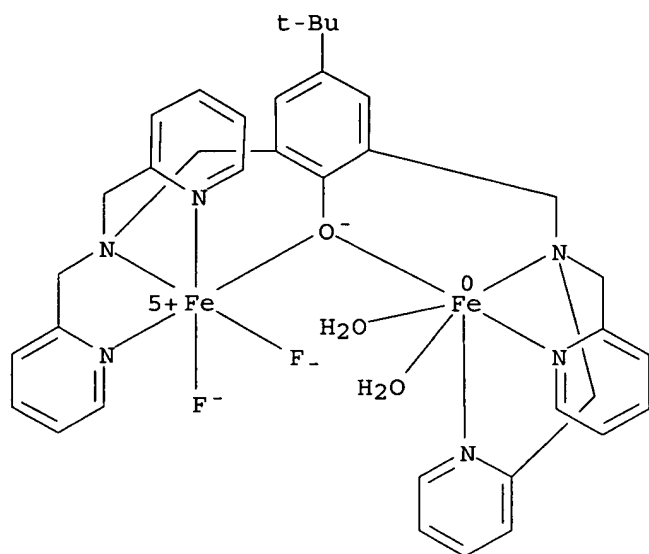
CM 2

CRN 202129-00-8

CMF C36 H43 F2 Fe2 N6 O3

CCI CCS



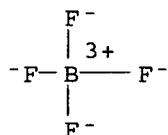


CM 3

CRN 14874-70-5

CMF B F4

CCI CCS



RN 202129-05-3 CAPLUS

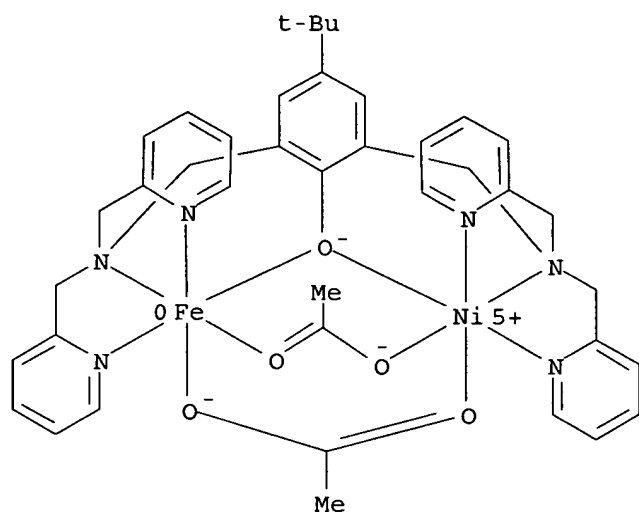
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]] (nickel)-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 202129-04-2

CMF C40 H45 Fe N6 Ni O5

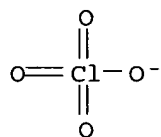
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 202129-07-5 CAPLUS

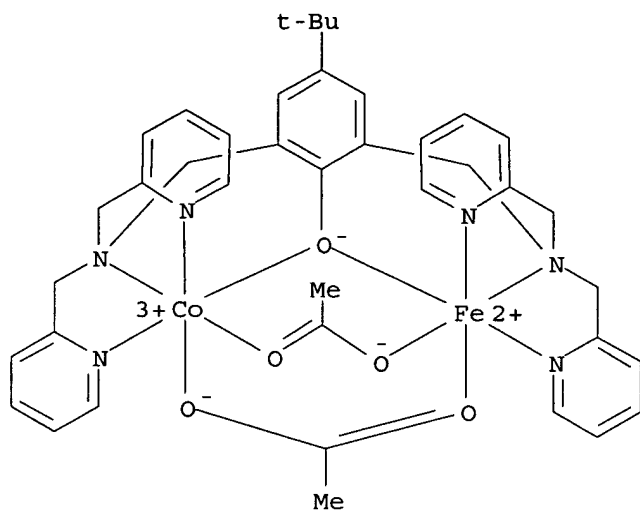
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]] (cobalt)-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 202129-06-4

CMF C40 H45 Co Fe N6 O5

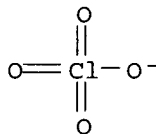
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 246234-27-5 CAPLUS

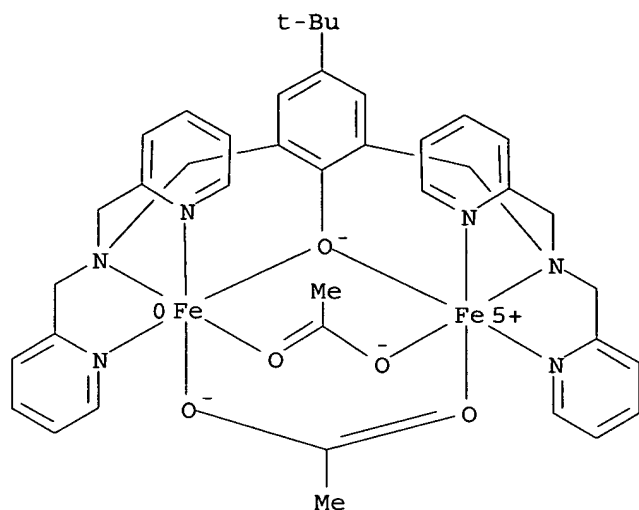
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]]di-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 246143-98-6

CMF C40 H45 Fe2 N6 O5

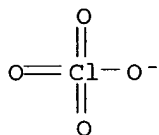
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



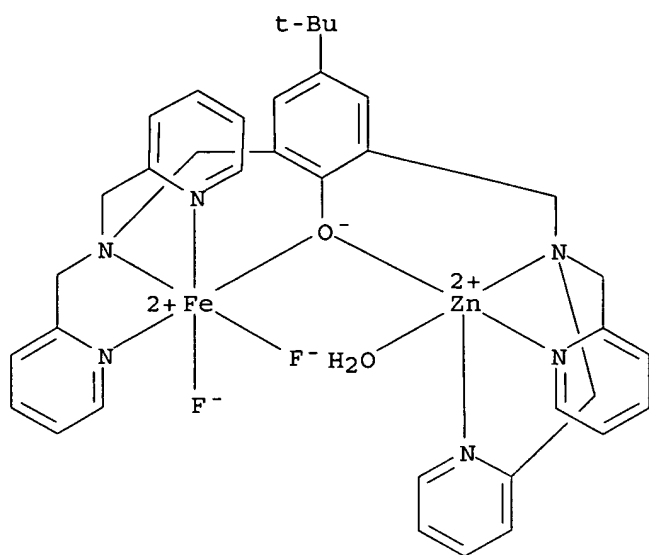
IT 246144-00-3 246144-01-4 246144-02-5

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(elec. potential of couple containing)

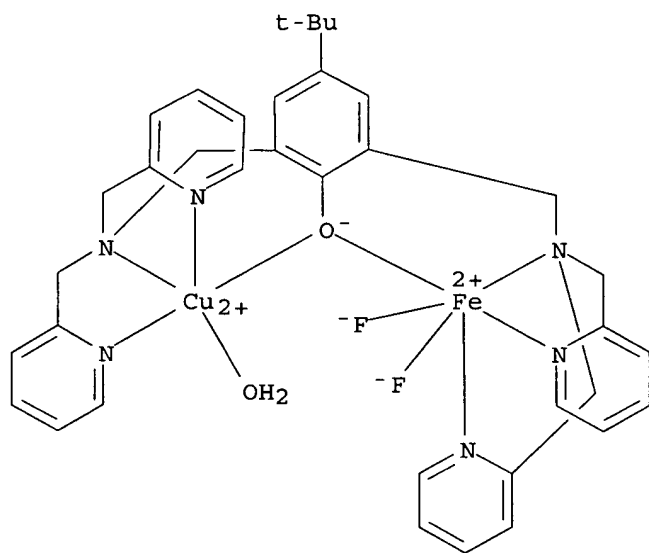
RN 246144-00-3 CAPLUS

CN Iron(1+), (aquazinc) [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato- $\kappa$ O: $\kappa$ O]]difluoro-, stereoisomer (9CI) (CA INDEX NAME)



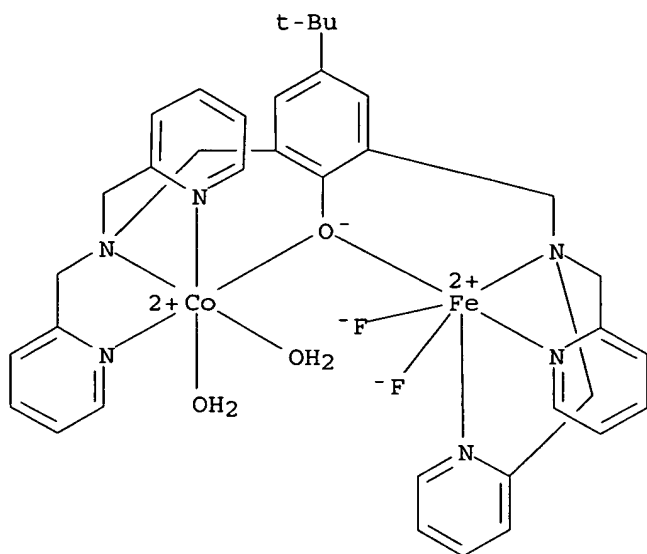
RN 246144-01-4 CAPLUS

CN Iron(1+), (aquacopper) [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato- $\kappa$ O: $\kappa$ O]]difluoro-, stereoisomer (9CI) (CA INDEX NAME)



RN 246144-02-5 CAPLUS

CN Iron(1+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato- $\kappa$ O: $\kappa$ O]](diaquacobalt)difluoro-, stereoisomer (9CI) (CA INDEX NAME)



IT 246144-06-9

RL: PRP (Properties)

(ferromagnetic coupling of)

RN 246144-06-9 CAPLUS

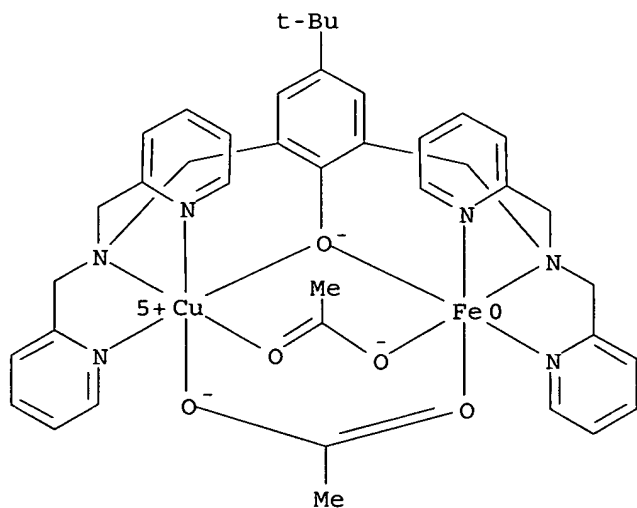
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]] (copper)-, stereoisomer, bis[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 246144-05-8

CMF C40 H45 Cu Fe N6 O5

CCI CCS

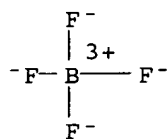


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

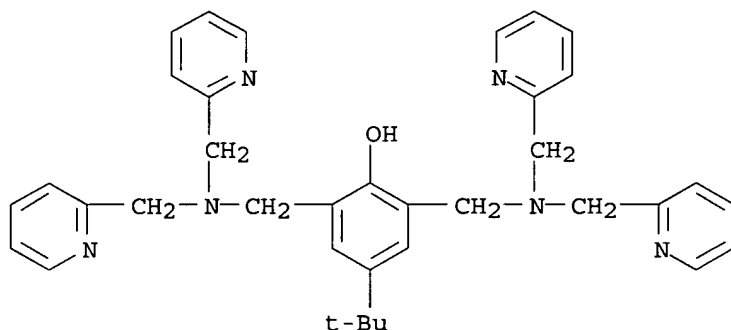


IT 202128-99-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of iron homo- and heterodinuclear **difluoro** phenol derivative aqua complexes as acid **phosphatase** active site models)

RN 202128-99-2 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-(1,1-dimethylethyl)-  
(9CI) (CA INDEX NAME)

IT 246143-99-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, crystal structure and Mossbauer effect of)

RN 246143-99-7 CAPLUS

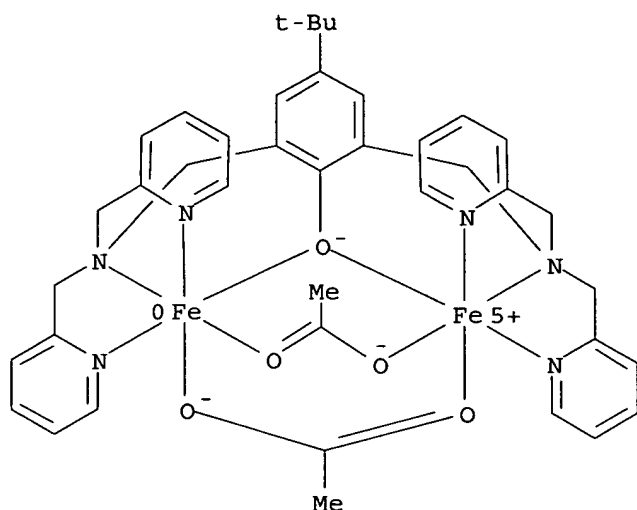
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN]methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]]di-, stereoisomer,  
bis[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 246143-98-6

CMF C40 H45 Fe2 N6 O5

CCI CCS

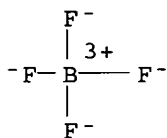


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 246143-94-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, crystal structure, electrochem. magnetic properties of iron  
 homo- and heterodinuclear **difluoro**  
 butylbis[bis(pyridylmethyl)aminomethyl]phenol aqua complexes as acid  
**phosphatase** active site models)

RN 246143-94-2 CAPLUS

CN Iron(2+), (aquacopper) [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl-  
 $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato-  
 $\kappa$ O: $\kappa$ O]]difluoro-, stereoisomer, bis[tetrafluoroborate(1-)],  
 tetrahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 246143-93-1

CMF C36 H41 Cu F2 Fe N6 O2 . 2 B F4

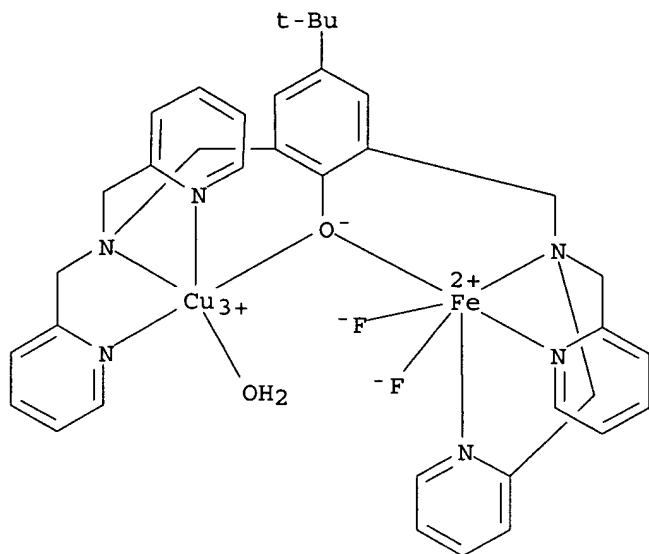
CM 2

CRN 246143-92-0

CMF C36 H41 Cu F2 Fe N6 O2

CCI CCS



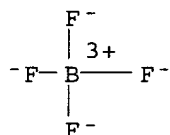


CM 3

CRN 14874-70-5

CMF B F4

CCI CCS



IT 246143-91-9P 246143-97-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, electrochem., magnetic and structural properties of iron homo-  
 and heterodinuclear difluoro butylbis(bis(pyridylmethyl)amino  
 methyl]phenol aqua complexes as acid **phosphatase** active site  
 models)

RN 246143-91-9 CAPLUS

CN Iron(2+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino-  
 $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato-  
 $\kappa$ O: $\kappa$ O]](diaquacobalt)difluoro-, stereoisomer,  
 bis[tetrafluoroborate(1-)], hydrate (2:5) (9CI) (CA INDEX NAME)

CM 1

CRN 246143-90-8

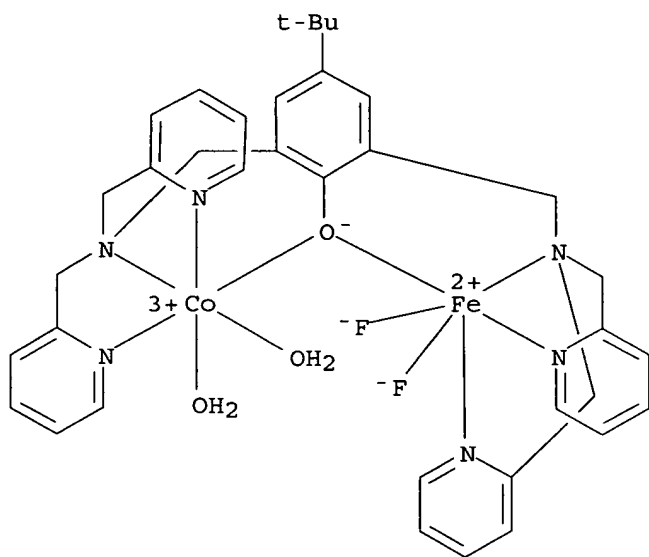
CMF C36 H43 Co F2 Fe N6 O3 . 2 B F4

CM 2

CRN 246143-89-5

CMF C36 H43 Co F2 Fe N6 O3

CCI CCS

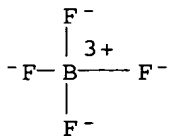


CM 3

CRN 14874-70-5

CMF B F4

CCI CCS



RN 246143-97-5 CAPLUS

CN Iron(2+), (aquazinc) [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato- $\kappa$ O: $\kappa$ O]]difluoro-, stereoisomer, bis[tetrafluoroborate(1-)], hydrate (2:7) (9CI) (CA INDEX NAME)

CM 1

CRN 246143-96-4

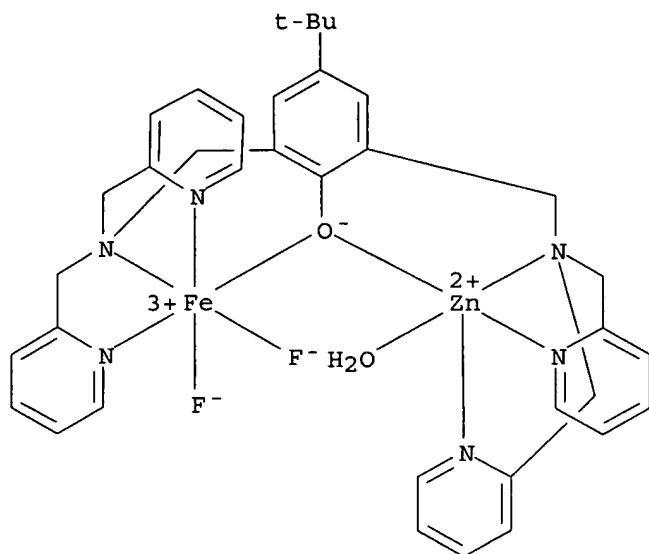
CMF C36 H41 F2 Fe N6 O2 Zn . 2 B F4

CM 2

CRN 246143-95-3

CMF C36 H41 F2 Fe N6 O2 Zn

CCI CCS

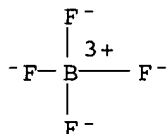


CM 3

CRN 14874-70-5

CMF B F4

CCI CCS



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 88 OF 52 CAPLUS> COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:640407 CAPLUS

DOCUMENT NUMBER: 129:272665

TITLE: High throughput assays using fusion proteins for screening binding compounds and protease inhibitors  
 INVENTOR(S): Hermes, Jeffrey D.; Salowe, Scott P.; Sinclair, Peter J.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------|------|----------|-----------------|----------|
| WO 9841866    | A1   | 19980924 | WO 1998-US4610  | 19980310 |
| W: CA, JP, US |      |          |                 |          |

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
PRIORITY APPLN. INFO.: US 1997-40795P P 19970314

- AB This application describes a high throughput assay for screening compds. which are capable of binding to a fusion protein which consists of a target protein and an FK506-binding protein. This application also describes an assay for screening compds. which inhibit a protease. A FK506-binding protein-ZAP70 tandem SH2 domains fusion protein was recombinantly prepared, expressed in Escherichia coli, and purified by affinity chromatog. on agarose-immobilized avidin having bound biotinylated **phosphopeptide** derived from the  $\zeta$ 1 ITAM sequence of the human T-cell receptor. Inhibitors of the fusion protein are screened using the **biotinylphosphopeptide**, the fusion protein, and europium cryptate-labeled FK506 analog in wells of a 96-well black microplate. The **fluorescence** ratio is measured in a Packard Discovery homogeneous time-resolved **fluorescence** analyzer.
- IC ICM G01N033-53  
ICS G01N033-544; G01N033-531
- CC 9-5 (Biochemical Methods)  
Section cross-reference(s): 3, 7, 15
- ST fusion protein binding compd screening; protease inhibitor screening  
fusion protein; FK506 binding protein **fluorescence** assay
- IT TCR (T cell receptors)  
RL: MSC (Miscellaneous)  
(ITAM (immunoreceptor tyrosine-based activation motif) sequence of, biotinylated **phosphopeptide** from, in fusion protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)
- IT Protein motifs  
(ITAM (immunoreceptor tyrosine-based activation motif), biotinylated **phosphopeptide** from, in fusion protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)
- IT **Phosphoproteins**  
RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(ZAP-70 (TCR receptor  $\zeta$ -chain-associated, 70,000-mol.-weight), SH2 domain, fusion protein containing, as target protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)
- IT Avidins  
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process); USES (Uses)  
(agarose-immobilized, complexes with biotinylated ITAM **phosphopeptide**, as affinity matrix for purification of fusion proteins; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)
- IT **Phosphopeptides**  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
(biotinylated, from ITAM sequence, in fusion protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)
- IT **Phosphoproteins**  
RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); BPR (Biological process); BSU (Biological study, unclassified); ANST

(Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(p72syk, SH2 domain, fusion protein containing, as target protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **Fluorometry**

(time-resolved; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **125433-96-7**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(FK506 analog labeled with, as donor-labeled ligands; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **188796-99-8**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(amino acid sequence, of human T-cell receptor Zeta 1, fusion protein containing; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **9012-36-6D, Agarose, avidin conjugates, complexes with biotinylated ITAM phosphopeptide 213611-43-9D, complexes with agarose-immobilized**

avidin 213611-44-0D, complexes with agarose-immobilized avidin  
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process); USES (Uses)

(as affinity matrix for purification of fusion proteins; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **79747-53-8, Tyrosine phosphatase**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(fusion protein containing, as target protein; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **146669-16-1**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(mol. containing, coupled to lanthanide, as donor-labeled ligands; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

IT **125433-96-7**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(FK506 analog labeled with, as donor-labeled ligands; high throughput assays using fusion proteins for screening binding compds. and protease inhibitors)

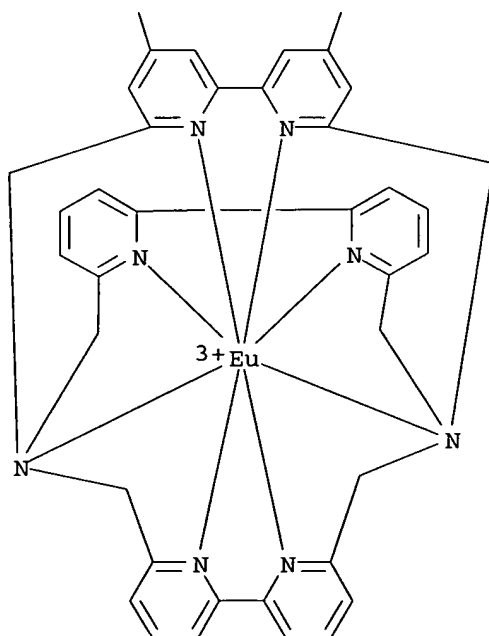
RN **125433-96-7 CAPLUS**

CN Europium(3+), [N,N'-bis(2-aminoethyl)-1,14,39,40,41,42,43,44-octaazaoctacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5,10-dicarboxamide-N1,N14,N39,N40,N41,N42,N43,N44]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



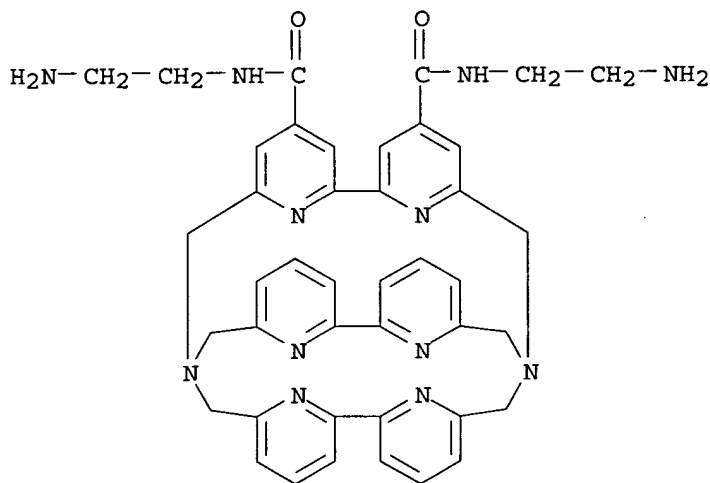
IT 146669-16-1

RL: ARG (Analytical reagent use); BPR (Biological process); BSU  
(Biological study, unclassified); ANST (Analytical study); BIOL

(Biological study); PROC (Process); USES (Uses)  
 (mol. containing, coupled to lanthanide, as donor-labeled ligands; high  
 throughput assays using fusion proteins for screening binding compds.  
 and protease inhibitors)

RN 146669-16-1 CAPLUS

CN 1,14,39,40,41,42,43,44-Octaazaocyclac[12.12.12.13,7.18,12.116,20.121,25.  
 128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(  
 41),28,30,32(40),33,35,37(39)-octadecaene-5,10-dicarboxamide,  
 N,N'-bis(2-aminoethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 39 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:589872 CAPLUS

DOCUMENT NUMBER: 129:285165

TITLE: Structure and Reactivity of Dinuclear Cobalt(III)  
 Complexes with Peroxide and **Phosphate**  
 Diester Analogs Bridging the Metal Ions

AUTHOR(S): Seo, Jin Seog; Hynes, Rosemary C.; Williams, Daniel;  
 Chin, Jik; Sung, Nack-Do

CORPORATE SOURCE: Department of Chemistry, McGill University, Montreal,  
 QC, H3A 2K6, Can.

SOURCE: Journal of the American Chemical Society (1998),  
 120(38), 9943-9944

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Understanding how 2 metal ions cooperatively hydrolyze **phosphate**  
 esters is currently a topic of much interest in chemical and biol. Metal  
 ion-catalyzed hydrolysis of **phosphate** diesters with poor leaving  
 groups is of particular interest since some of the mols. of life (DNA,

RNA, **phospholipids**) contain such linkages. Hydrolyzing **phosphate** diesters with poor leaving groups is exceptionally difficult as they are enormously more stable compared with **phosphate** diesters with good leaving groups. Because it has been suggested that metal-bound peroxides can be effective nucleophiles for cleaving **phosphates**, we examined the conversion of (I; X = OMe) to II. The structure of (I; X = Ph) was determined in this study as a model for the structure of (I; X = OMe), while the structure of II was determined previously. Replacing di-Ph **phosphinate** in the synthesis of (I; X = Ph) with Me **phosphonate** gave (I; X = OMe). Hydrolysis of the **phosphonate** ester bond in (I; X = OMe) was monitored by <sup>1</sup>H and <sup>31</sup>P NMR. The <sup>1</sup>H NMR of the product of hydrolysis of (I; X = OMe) matches that of a genuine sample of II prepared from **phenylphosphonate**. The pseudo-first-order rate constant for the hydrolysis of the ester bond in (I; X = OMe) was 5 x 10<sup>-7</sup>. In general **phosphate** monoesters are about as stable as **phosphate** diesters.

- CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 75
- ST crystal structure dicobalt pyridinylmethylaminomethylphenol peroxo **phosphinate**; cobalt pyridinylmethylaminomethylphenol peroxo **phosphinate phenylphosphonate** prepn; kinetics hydrolysis **phosphonate** ester cobalt dinuclear
- IT Hydrolysis  
Hydrolysis kinetics  
(of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo Me **phenylphosphinate** complex)
- IT Crystal structure  
Molecular structure  
(of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo di-Ph **phosphinate** complex)
- IT 7162-15-4, Methyl **phenylphosphinate**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for preparation of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo Me **phenylphosphinate** complex)
- IT 1707-03-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for preparation of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo di-Ph **phosphinate** complex)
- IT 184358-71-2  
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
(formation from hydrolysis of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo Me **phenylphosphonate** complex)
- IT 213818-45-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)
- IT 213818-43-0P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and kinetics of hydrolysis of)
- IT 184358-71-2  
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
(formation from hydrolysis of cobalt bis((bis(pyridinylmethyl)amino)methyl)methylphenol peroxo Me **phenylphosphonate** complex)
- RN 184358-71-2 CAPLUS
- CN Cobalt(2+), aqua[μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN]methyl]-4-methylphenolato-κO:κO]]hydroxy[μ-[phenylphosphonato(2-)-κO:κO']]di-, diperchlorate (9CI) (CA INDEX NAME)

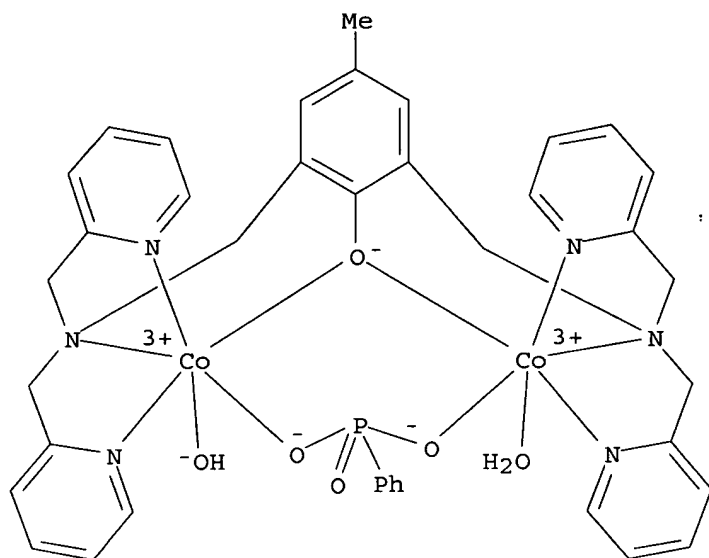


CM 1

CRN 184358-70-1

CMF C39 H41 Co2 N6 O6 P

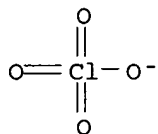
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 213818-45-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 213818-45-2 CAPLUS

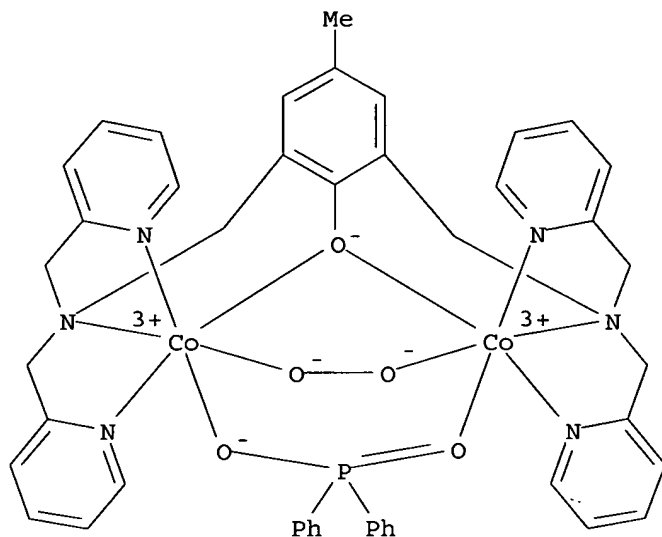
CN Cobalt(2+), [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-methylphenolato-κO:κO]] [μ-(diphenylphosphinato-κO:κO')] [μ-(peroxy-κO:κO')] di-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 213818-44-1

CMF C45 H43 Co2 N6 O5 P

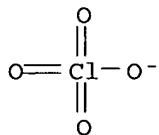
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 213818-43-0P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and kinetics of hydrolysis of)

RN 213818-43-0 CAPLUS

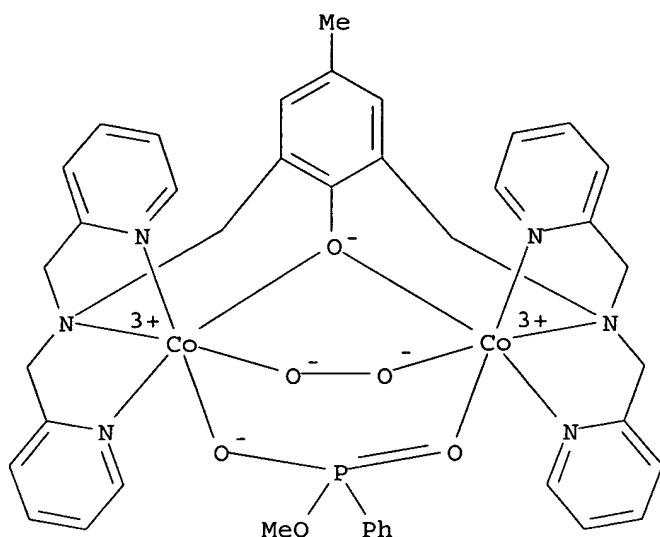
CN Cobalt(2+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]methyl]-4-methylphenolato- $\kappa$ O: $\kappa$ O]] [ $\mu$ -(monomethyl phenylphosphonato- $\kappa$ O': $\kappa$ O'')] [ $\mu$ -(peroxy- $\kappa$ O: $\kappa$ O')]di-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 213818-42-9

CMF C40 H41 Co2 N6 O6 P

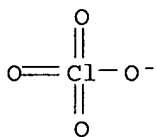
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 40 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:401835 CAPLUS

DOCUMENT NUMBER: 129:1B0485

TITLE: A new model for the reduced form of purple acid  
**phosphatase**: structure and properties of  
[Fe<sub>2</sub>BPLMP(OAc)<sub>2</sub>](BPh<sub>4</sub>)<sub>2</sub>

AUTHOR(S): Yim, Seon Hwa; Lee, Ho Jin; Lee, Kang-Bong; Kang,  
Seong Ju; Hur, Nam Hwi; Jang, Ho G.

CORPORATE SOURCE: Department of Chemistry, Korea University, Seoul,  
136-701, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (1998), 19(6),  
654-660

CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB [Fe<sub>2</sub>BPLMP(OAc)<sub>2</sub>](BPh<sub>4</sub>)<sub>2</sub> (1), a new model for the reduced form of the purple acid **phosphatases**, was synthesized by using a dinucleating ligand, 2,6-bis[(2-pyridylmethyl)(6-methyl-2-pyridylmethyl)amino)methyl]-4-methylphenol (HBPLMP). Complex 1 was characterized by x-ray diffraction as having a (μ-

phenoxo)bis(acetato)diiron core. Complex 1 was crystallized in the monoclinic space group C2/c with the following cell parameters: a 41.620(6), b 14.020(3), c 27.007(4) Å,  $\beta$  90.60(2)°, and Z = 8. The iron centers in complex 1 are ordered as indicated by the difference in the Fe-O bond lengths which match well with typical FeIII-O and FeII-O bond lengths. Complex 1 was studied by electronic spectral, NMR, EPR, SQUID, and electrochem. methods. Complex 1 exhibits strong bands at 592 nm and 1380 nm in CH<sub>3</sub>CN ( $\epsilon$ =1.0 + 10<sup>3</sup>, 3.0 + 10<sup>2</sup>). These are assigned to phenolate-to-FeIII and intervalence charge-transfer transitions, resp. Its NMR spectrum exhibits sharp isotropically shifted resonances, which are half of those expected for a valence-trapped species, indicating that electron transfer between FeII and FeIII centers is faster than NMR time scale. This complex undergoes quasireversible 1-electron redox processes. The FeIII<sub>2</sub>/FeIIFeIII and FeIIFeIII/FeII<sub>2</sub> redox couples are at 0.655 and -0.085 V vs. SCE, resp. It has K<sub>comp</sub>=3.3 + 10<sup>12</sup> representing that BPLMP/bis(acetate) ligand combination stabilizes a mixed-valence FeIIFeIII complex in the air. Complex 1 exhibits a broad EPR signal centered near g = 1.55 which is a characteristic feature of the antiferromagnetically coupled high-spin FeIIFeIII system (S<sub>total</sub> = 1/2). This is consistent with the magnetic susceptibility study showing the weak antiferromagnetic coupling (J = -4.6 cm<sup>-1</sup>, H = -2JS<sub>1</sub>·S<sub>2</sub>) between FeII and FeIII centers.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 7, 72, 75, 77

ST crystal structure iron pyridylmethylaminomethylphenolato acetato dinuclear; iron pyridylmethylaminomethylphenolato acetato dinuclear prepn structure; phenolate pyridylmethylaminomethyl iron dinuclear prepn structure; magnetic property iron pyridylmethylaminomethylphenolato acetato dinuclear; antiferromagnetic coupling iron pyridylmethylaminomethylphenolato acetato dinuclear; electrochem redox iron pyridylmethylaminomethylphenolato acetato dinuclear; electron transfer iron pyridylmethylaminomethylphenolato acetato dinuclear; purple acid **phosphatase** model iron pyridylmethylaminomethylphenolato

IT Enzyme functional sites

(active; iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

IT Redox reaction

(electrochem.; of iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

IT Antiferromagnetic exchange

Charge transfer transition

Crystal structure

ESR (electron spin resonance)

Magnetic susceptibility

Molecular structure

(of iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

IT 1122-72-1, 6-Methyl-2-pyridinecarboxaldehyde 3731-51-9,  
2-(Aminomethyl)pyridine 5862-32-8, 2,6-Bis(chloromethyl)-4-methylphenol  
RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

IT 210175-87-4P, 2,6-Bis(((2-pyridylmethyl)(6-methyl-2-pyridylmethyl)amino)methyl)-4-methylphenol 210175-88-5P,  
(2-Pyridylmethyl)(6-methyl-2-pyridylmethyl)amine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(for preparation of iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

IT **210175-86-3P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, crystal structure, electrochem. redox and magnetic properties as model of reduced purple acid **phosphatase**)

IT 9001-77-8, Acid **phosphatase**

RL: PRP (Properties)

(reduced purple; iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

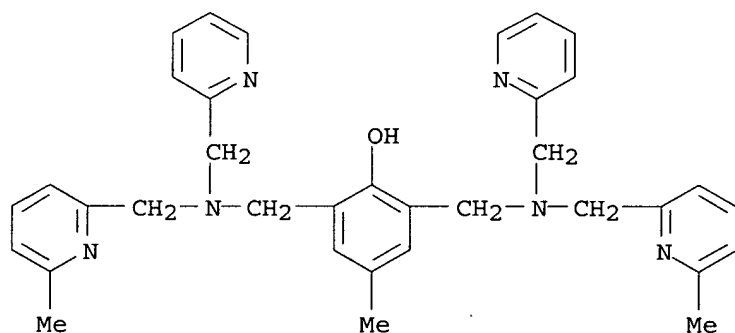
IT **210175-87-4P**, 2,6-Bis[((2-pyridylmethyl)(6-methyl-2-pyridylmethyl)amino)methyl]-4-methylphenol

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of iron bis((pyridylmethyl)(methylpyridylmethyl)aminomethyl)methylphenolato acetato dinuclear complex as model of reduced purple acid **phosphatase**)

RN 210175-87-4 CAPLUS

CN Phenol, 4-methyl-2,6-bis[[[(6-methyl-2-pyridinyl)methyl](2-pyridinylmethyl)amino)methyl]- (9CI) (CA INDEX NAME)



IT **210175-86-3P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, crystal structure, electrochem. redox and magnetic properties as model of reduced purple acid **phosphatase**)

RN 210175-86-3 CAPLUS

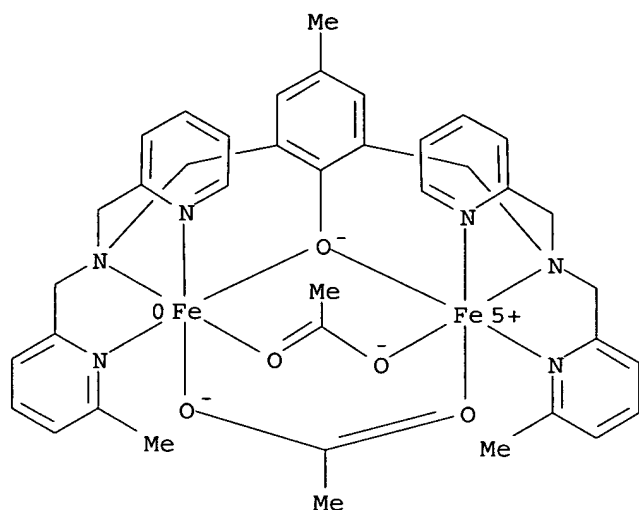
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[4-methyl-2,6-bis[[[(6-methyl-2-pyridinyl-κN)methyl][(2-pyridinyl-κN)methyl]amino-κN)methyl]phenolato-κO:κO]] di-, stereoisomer, bis[tetraphenylborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 210175-85-2

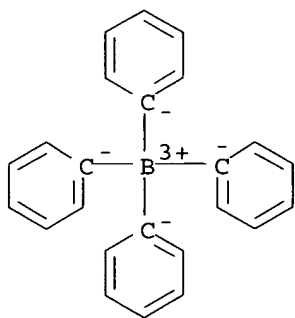
CMF C39 H43 Fe2 N6 O5

CCI CCS



CM 2

CRN 4358-26-3  
 CMF C24 H20 B  
 CCI CCS



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 41 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1997:737577 CAPLUS  
 DOCUMENT NUMBER: 128:125231  
 TITLE: Dinuclear iron(III)-metal(II) complexes as structural core models for purple acid **phosphatases**  
 AUTHOR(S): Ghiladi, Morten; McKenzie, Christine J.; Meier, Anke; Powell, Annie K.; Ulstrup, Jens; Wocadlo, Sigrid  
 CORPORATE SOURCE: Department of Chemistry, Odense University, Odense M, DK-5230, Den.  
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1997), (21), 4011-4018  
 CODEN: JCDBTI; ISSN: 0300-9246  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of mixed-valent iron and mixed-metal FeIII-MII (M = Zn, Cu, Ni or Co) complexes of the phenolate-hinged dinucleating ligand 2,6-bis{[bis(2-pyridylmethyl)amino]methyl}-4-tert-butylphenolato(1-), bpbp- have been prepared and characterized. Both exogenous bidentate bridging groups and different terminal ligands bound to each different metal ion at the exogenous site were identified. The structure of the mixed-valence complex [(bpbp)Fe<sub>2</sub>(F)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>][BF<sub>4</sub>]<sub>2</sub> confirms that it is a rare example of a dimetallic complex of a single-atom hinged acyclic dinucleating ligand with a 'non-bridged' arrangement at the exogenous bridging site. Mossbauer spectroscopy indicates valence trapping in this complex with the parameters,  $\Delta E_Q$  3.242 mm s<sup>-1</sup>,  $\delta$  1.169 mm s<sup>-1</sup> and  $\Delta E_Q$  0.221 mm s<sup>-1</sup>,  $\delta$  0.460 mm s<sup>-1</sup>, resp. for the high spin Fe<sup>2+</sup> and high spin Fe<sup>3+</sup> ions. Crystals of [(bpbp)Fe<sub>2</sub>(F)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>][BF<sub>4</sub>]<sub>2</sub>.cnt dot.4H<sub>2</sub>O are triclinic, space group P<sub>2</sub>1/n (number 2), with a = 12.695(1), b = 19.197(2), c = 10.202(1) Å,  $\alpha$  = 102.95(1),  $\beta$  = 97.61(1),  $\gamma$  = 93.76(1)°, Z = 2. The structure was refined to R = 0.1009 on F using 4338 reflections with I > 2 $\sigma$ (I) (wR<sub>2</sub> on all data and F<sub>2</sub> = 0.3522). The FeII and FeIII atoms are bridged asym. by the phenolic oxygen atom of bpbp- with FeII-O 2.175(6) Å and FeIII-O 2.033(6) Å with a FeIII...FeII distance of 3.726(2) Å. The two terminal **fluoride** ions are bound to the FeIII atom and strongly hydrogen bonded to two water mols. bound to the adjacent FeII atom. This complex may model the mode in which **fluoride** ions bind to the active site of the purple acid **phosphatases** (PAPs) thereby inhibiting the activity of these enzymes. Tetrahedral oxo anions are known also to inhibit PAPs and to mimic this inhibition a FeIII-ZnII complex incorporating molybdate bridging groups was prepared. Crystals of [(bpbp)FeZn(MoO<sub>4</sub>)<sub>2</sub>].C<sub>3</sub>H<sub>7</sub>OH. cntdot.2H<sub>2</sub>O are monoclinic, space group P<sub>2</sub>1/n with a = 11.773(13), b = 21.394(7), c = 17.001(11) Å and  $\beta$  = 90.98(7)°, Z = 4. The structure was refined to R = 0.0434 on F using 3758 reflections with I > 2 $\sigma$ (I) (wR<sub>2</sub> on all data and F<sub>2</sub> = 0.1339). The FeIII...ZnII distance is 3.819(4) Å. A series of acetate-bridged complexes were prepared by the novel method of diffusing Et acetate or iso-Pr acetate into mixts. of Hbpbp and iron perchlorate in the presence and absence of second type of metal ion. The acetate bridging groups are the result of the hydrolysis of the alkyl acetate. These complexes have the general formulation [(bpbp)FeM(CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>][ClO<sub>4</sub>]<sub>2</sub>. Crystals of [(bpbp)FeCu(CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>][ClO<sub>4</sub>]<sub>2</sub>.0.5CH<sub>3</sub>OH are monoclinic, space group P<sub>2</sub>1/n with a = 12.677(2), b = 22.059(2), c = 16.269(2) Å and  $\beta$  = 94.184(1)°, Z = 4. The structure was refined to R = 0.0538 on F using 5097 reflections with I > 2 $\sigma$ (I) (wR<sub>2</sub> on all data and F<sub>2</sub> = 0.2684). The FeIII...CuII distance is 3.419(2) Å. Asym. bridging by the hinging phenolate group is evident in the bis(molybdate)-bridged Fe-Zn complex and the bis(acetate)-bridged Fe-Cu complex, however it is significantly less pronounced compared with the 'non-bridged' **fluoride** containing FeIII-FeII complex. While the **fluoride** and molybdate complexes may model aspects of the binding of these ions in inhibited PAPs, the generation of acetate complexes from the hydrolysis of alkyl esters may indeed model part of the reactivity of PAPs. However, we have unfortunately not been able to ascertain that this reaction is promoted by the metal complexes.

CC 7-4 (Enzymes)

Section cross-reference(s): 75

ST model purple acid **phosphatase**; iron metal complex prepn crystal structure

IT Crystal structure  
(preparation and crystal structure of dinuclear iron(III)-metal(II) complexes, structural core models for purple acid **phosphatases**)

IT 9001-77-8  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (model; preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

IT 202129-03-1 202129-05-3 202129-07-5  
 202129-09-7  
 RL: PRP (Properties)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

IT 202129-01-9P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

IT 98-54-4, 4-tert-Butylphenol 1539-42-0, N,N-Bis(2-pyridylmethyl)amine  
 10025-64-6 13877-16-2 30525-89-4, Paraformaldehyde 55144-08-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

IT 202128-99-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

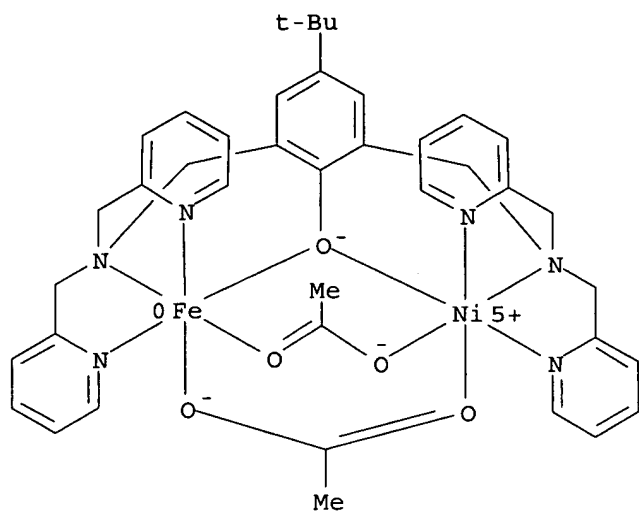
IT 202129-05-3 202129-07-5 202129-09-7  
 RL: PRP (Properties)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

RN 202129-05-3 CAPLUS  
 CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-  
 pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-  
 dimethylethyl)phenolato-κO:κO]] (nickel)-, stereoisomer,  
 diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 202129-04-2  
 CMF C40 H45 Fe N6 Ni O5  
 CCI CCS

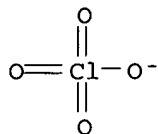




CM 2

CRN 14797-73-0

CMF Cl O4



RN 202129-07-5 CAPLUS

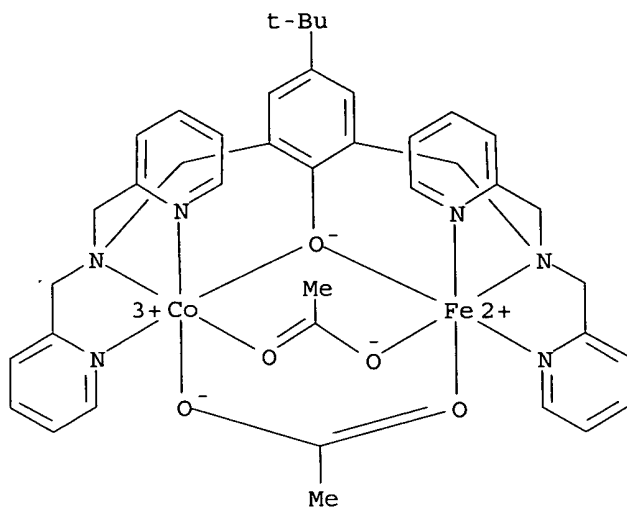
CN Iron(2+), bis[μ-(acetato-κO:κO')] [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-(1,1-dimethylethyl)phenolato-κO:κO]] (cobalt)-, stereoisomer, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 202129-06-4

CMF C40 H45 Co Fe N6 O5

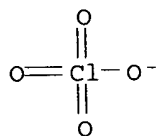
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 202129-09-7 CAPLUS

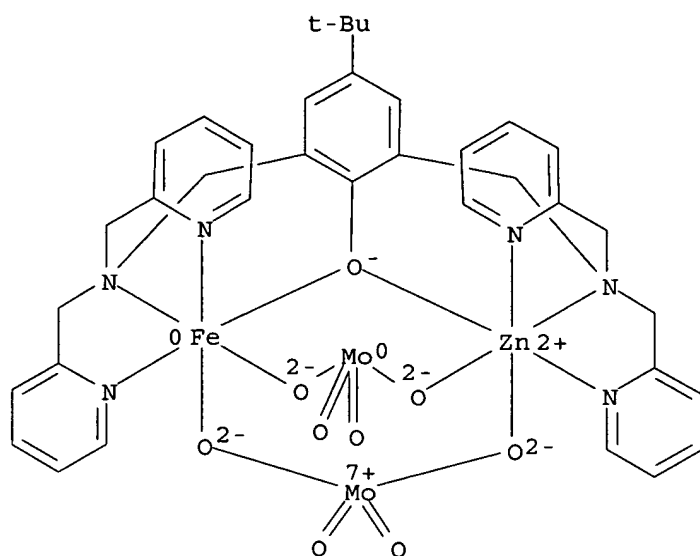
CN Molybdenum, [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(1,1-dimethylethyl)phenolato- $\kappa$ O: $\kappa$ O]](iron)tetra- $\mu$ -oxotetraoxo(zinc)di-, compd. with methanol (1:1), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 202129-08-6

CMF C36 H39 Fe Mo2 N6 O9 Zn

CCI CCS



CM 2

CRN 67-56-1

CMF C H4 O

H<sub>3</sub>C-OH

IT 202129-01-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of dinuclear iron(III)-metal(II)  
 complexes, structural core models for purple acid **phosphatases**  
 )

RN 202129-01-9 CAPLUS

CN Iron(2+), diaqua[μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-  
 κN)methyl]-4-(1,1-dimethylethyl)phenolato-  
 κO:κO]]difluorodi-, stereoisomer, bis[tetrafluoroborate(1-)],  
 tetrahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 246144-03-6

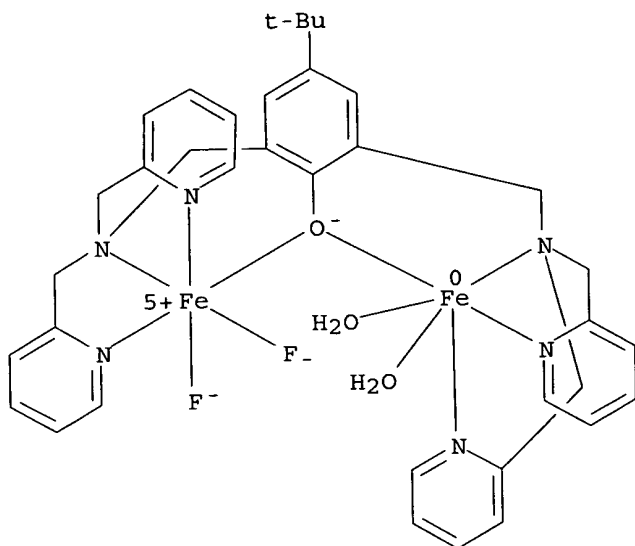
CMF C36 H43 F2 Fe2 N6 O3 . 2 B F4

CM 2

CRN 202129-00-8

CMF C36 H43 F2 Fe2 N6 O3

CCI CCS

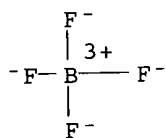


CM 3

CRN 14874-70-5

CMF B F4

CCI CCS



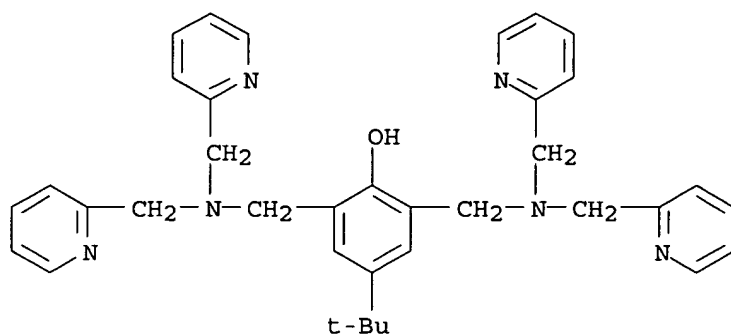
IT 202128-99-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and crystal structure of dinuclear iron(III)-metal(II) complexes, structural core models for purple acid phosphatases)

RN 202128-99-2 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L79 ANSWER 42 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:136918 CAPLUS

DOCUMENT NUMBER: 126:232631

TITLE: Stable Cu<sup>+</sup>, Ag<sup>+</sup> complexes of aza-bridged macrocyclic molecules: structure and chemical properties  
 AUTHOR(S): Takemura, Hiroyuki; Kon, Noriyoshi; Tani, Keita; Takehara, Ko; Kimoto, Junko; Shinmyozu, Teruo; Inazu, Takahiko

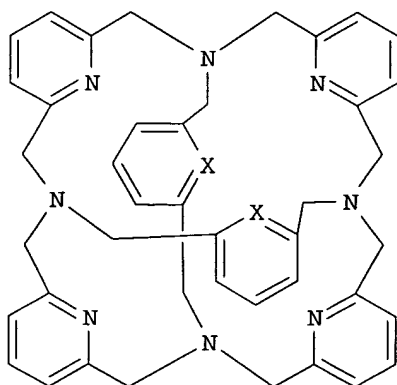
CORPORATE SOURCE: Dep. Chem., Kyushu Univ., Fukuoka, 810, Japan  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (3), 239-246

CODEN: JCPRB4; ISSN: 0300-922X  
 PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB The cage type compds. (I, X = CH 1; X = N 2) form stable Cu<sup>+</sup> or Ag<sup>+</sup> complexes, which were employed for the preparation of cation-free host mols. A reaction between the potassium complex K<sup>+</sup>c1 and a CuII salt generates a CuI complex. The CuII/CuI redox potential is observed at +0.43 V (vs. SCE) in the cyclic voltammetry, which shows that the Cu<sup>+</sup> state is stabilized by its rigid mol. skeleton and spatially fixed coordination sites. A reaction between Ag<sup>+</sup> and K<sup>+</sup>c2 yields the dinuclear complex 2Ag<sup>+</sup>c2, which x-ray crystallog. (triclinic, space group P.hivin.1, R

= 0.032) revealed to have a short Ag<sup>+</sup>...Ag<sup>+</sup> distance (2.78 Å). The halide anions (Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>) remove one Ag<sup>+</sup> from 2Ag<sup>+</sup>+c2 to give Ag<sup>+</sup>+c2, but further demetalation does not occur. CV measurements show that these silver complexes are electrochem. stable. Both silver complexes are stable to sunlight. The 1st preps. of guest-free hosts were achieved by treating Cu<sup>+</sup>+c1 or 2Ag<sup>+</sup>+c2 with CN<sup>-</sup>. Inclusions of neutral guests (NH<sub>3</sub>, BH<sub>3</sub>) were attempted using these guest-free hosts.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 72, 75

IT 188108-26-1

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(elec. potential of couple containing)

IT 64443-05-6, Tetrakis(acetonitrile)copper(1+) **hexafluorophosphate**

188108-24-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of copper pyridyl aza-bridged macrocyclic cryptand complex)

IT 188108-29-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of silver pyridyl aza-bridged macrocyclic cryptand complex)

IT 188108-28-3

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(formation and electrochem. redox)

IT 132233-45-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(guest-free preparation from copper pyridyl aza-bridged macrocyclic cryptand complex)

IT 115848-25-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(guest-free preparation from silver pyridyl aza-bridged macrocyclic cryptand complex and attempted inclusion of ammonia and borane)

IT 188108-22-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and electrochem. redox)

IT 188108-19-2P 188108-23-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 188108-21-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, crystal structure and demetalation by halides or tetrabutylammonium cyanide)

IT 188108-18-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, electrochem. oxidation and demetalation by tetrabutylammonium cyanide)

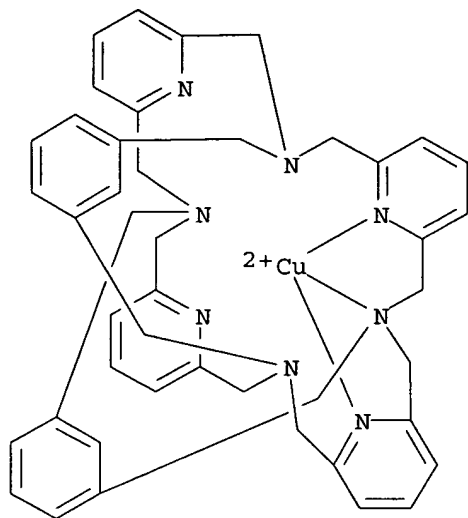
IT 188108-26-1

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(elec. potential of couple containing)

RN 188108-26-1 CAPLUS

CN Copper(2+), (1,9,17,25,40,41,49,51-octaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN40,κN41)-(9CI) (CA INDEX NAME)



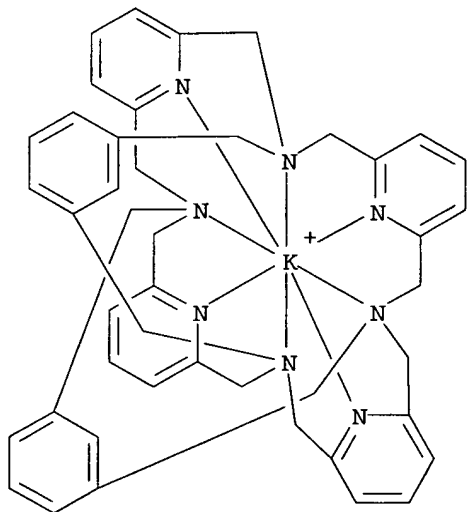
IT 188108-24-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of copper pyridyl aza-bridged macrocyclic cryptand complex)

RN 188108-24-9 CAPLUS

CN Potassium(1+), (1,9,17,25,40,41,49,51-octaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN9,κN17,κN25,κN40,κN41,κN49,κN51)-, bromide (9CI) (CA INDEX NAME)

● Br<sup>-</sup>

IT 188108-29-4

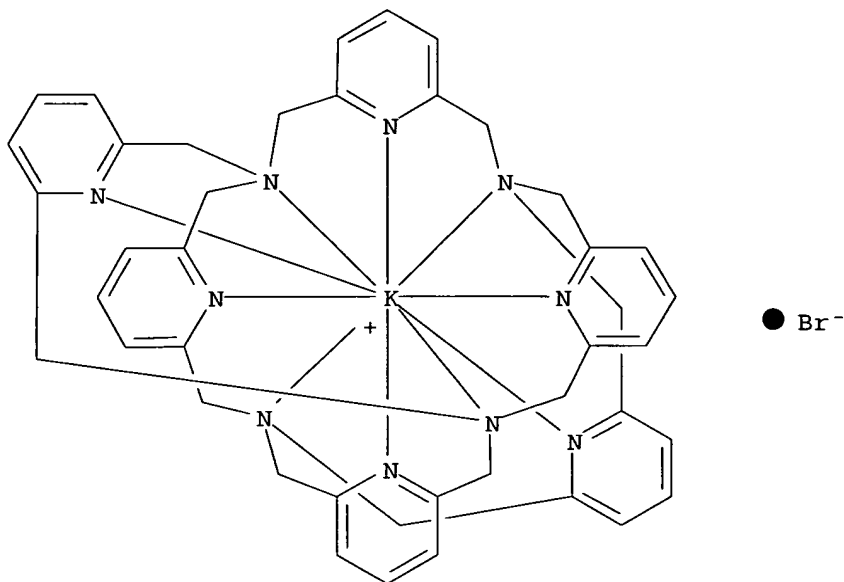
RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of silver pyridyl aza-bridged macrocyclic cryptand complex)

RN 188108-29-4 CAPLUS

CN Potassium(1+), (1,9,17,25,40,41,49,50,51,52-decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-

3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49) -  
 octadecaene- $\kappa$ N1, $\kappa$ N9, $\kappa$ N17, $\kappa$ N25, $\kappa$ N40, $\kappa$ N4  
 1, $\kappa$ N49, $\kappa$ N50, $\kappa$ N51, $\kappa$ N52)-, bromide (9CI) (CA INDEX  
 NAME)



IT 188108-28-3

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (formation and electrochem. redox)

RN 188108-28-3 CAPLUS

CN Silver(1+), (1,9,17,25,40,41,49,50,51,52-decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49) - octadecaene- $\kappa$ N1, $\kappa$ N9, $\kappa$ N17, $\kappa$ N25, $\kappa$ N40, $\kappa$ N41, $\kappa$ N49, $\kappa$ N50, $\kappa$ N51, $\kappa$ N52)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

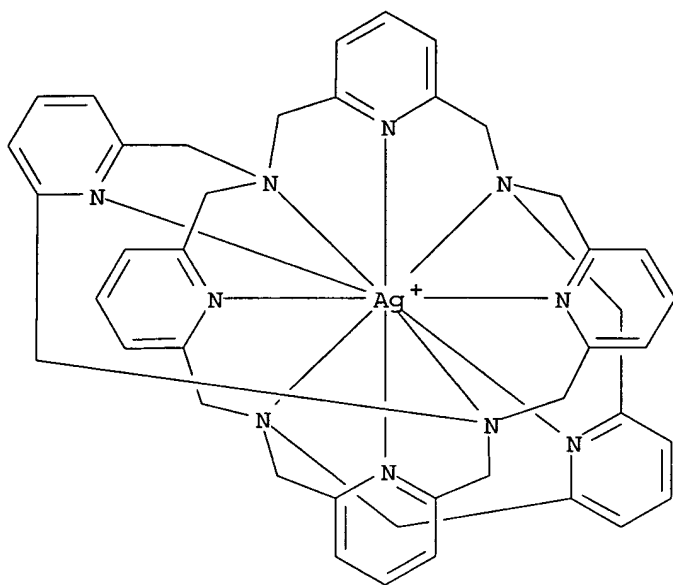
CM 1

CRN 188108-27-2

CMF C42 H42 Ag N10

CCI CCS



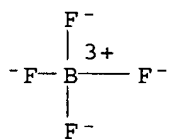


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



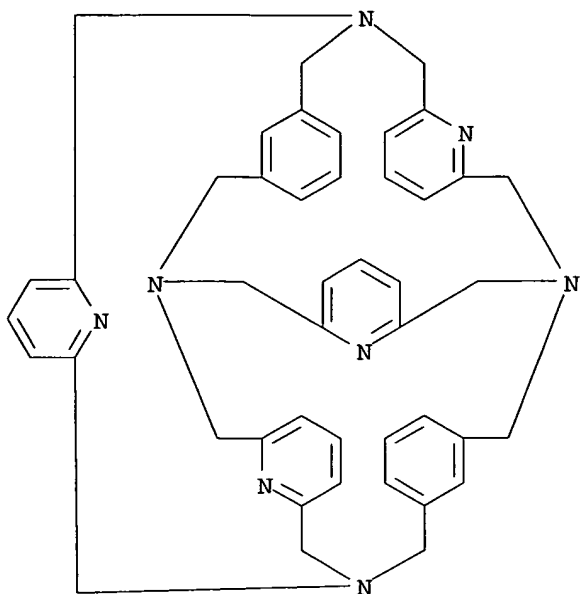
IT 132233-45-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(guest-free preparation from copper pyridyl aza-bridged macrocyclic cryptand complex)

RN 132233-45-5 CAPLUS

CN 1,9,17,25,40,41,49,51-Octaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.12  
7,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,  
31(41),34,36,38(40),43,45,47(49)-octadecaene (9CI) (CA INDEX NAME)



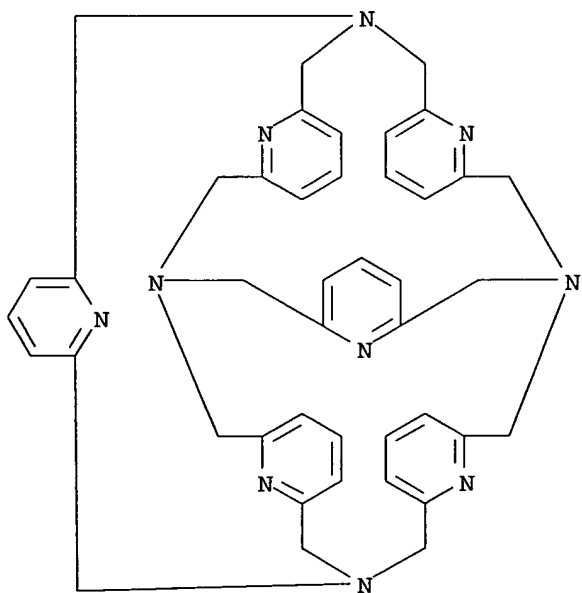
IT **115848-25-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(guest-free preparation from silver pyridyl aza-bridged macrocyclic cryptand complex and attempted inclusion of ammonia and borane)

RN 115848-25-4 CAPLUS

CN 1,9,17,25,40,41,49,50,51,52-Decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene (9CI) (CA INDEX NAME)



IT **188108-22-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and electrochem. redox)

RN 188108-22-7 CAPLUS

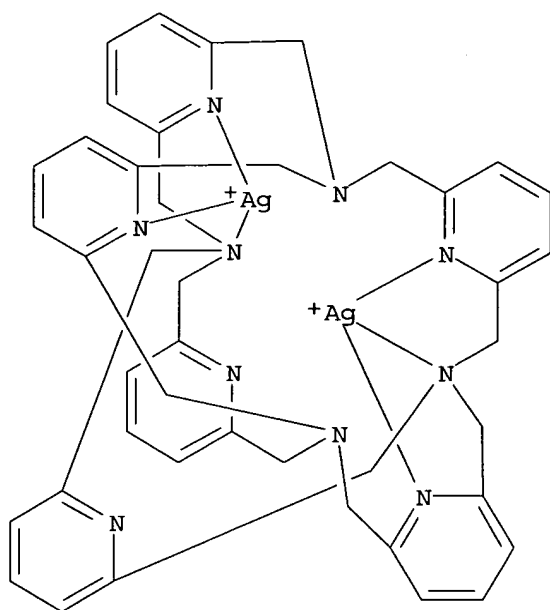
CN Silver(2+), [μ-(1,9,17,25,40,41,49,50,51,52-decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN40,κN41:κN9,κN50,κN51)]di-, dinitrate (9CI) (CA INDEX NAME)

CM 1

CRN 188108-20-5

CMF C42 H42 Ag2 N10

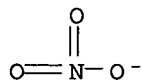
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3

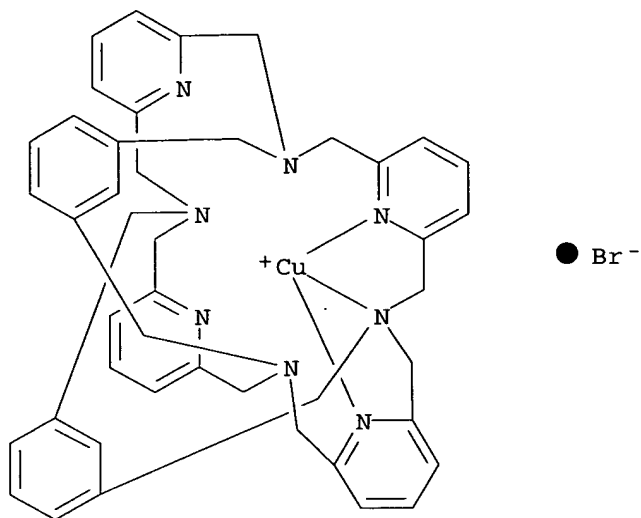


IT 188108-19-2P 188108-23-8P

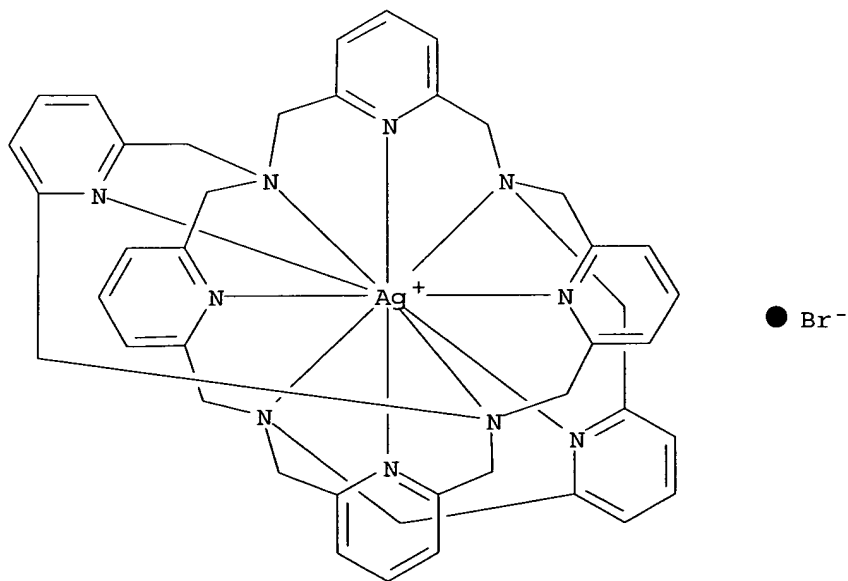
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 188108-19-2 CAPLUS

CN Copper(1+), (1,9,17,25,40,41,49,51-octaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN40,κN41)-, bromide (9CI) (CA INDEX NAME)



RN 188108-23-8 CAPLUS  
 CN Silver(1+), (1,9,17,25,40,41,49,50,51,52-decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN9,κN17,κN25,κN40,κN41,κN49,κN50,κN51,κN52)-, bromide (9CI) (CA INDEX NAME)

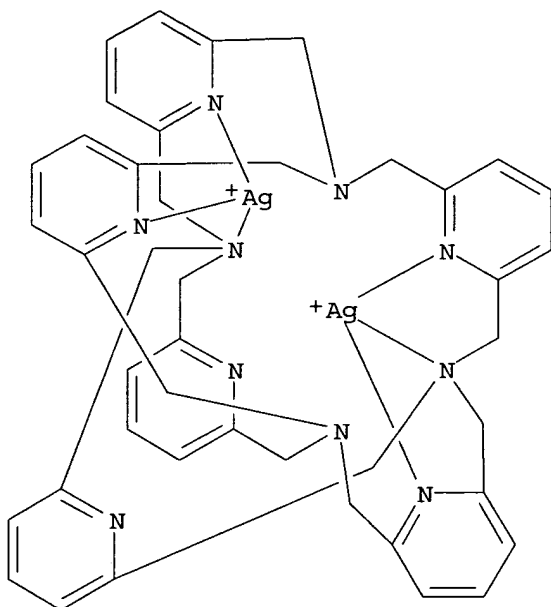


IT 188108-21-6P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, crystal structure and demetalation by halides or tetrabutylammonium cyanide)

RN 188108-21-6 CAPLUS  
 CN Silver(2+), [μ-(1,9,17,25,40,41,49,50,51,52-decaazanonacyclo[15.15.7.79,25.13,7.111,15.119,23.127,31.134,38.143,47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-κN1,κN40,κN41:κN9,κN50,κN51)]di-, bis[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

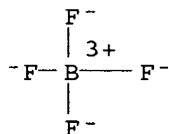
CM 1

CRN 188108-20-5  
 CMF C42 H42 Ag2 N10  
 CCI CCS



CM 2

CRN 14874-70-5  
 CMF B F4  
 CCI CCS



IT 188108-18-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, electrochem. oxidation and demetalation by tetrabutylammonium cyanide)  
 RN 188108-18-1 CAPLUS  
 CN Copper(1+), (1,9,17,25,40,41,49,51-octaazanonacyclo[15.15.7.79,25.13,7.111

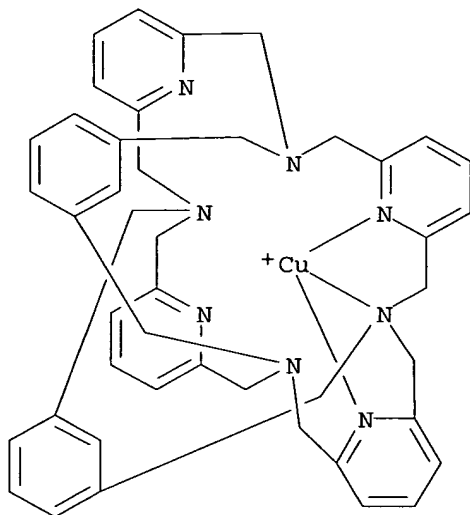
, 15.119, 23.127, 31.134, 38.143, 47]dopentaconta-3,5,7(52),11,13,15(51),19,21,23(50),27,29,31(41),34,36,38(40),43,45,47(49)-octadecaene-  
κN1,κN40,κN41)-, hexafluorophosphate(1-) (9CI) (CA  
INDEX NAME)

CM 1

CRN 188108-17-0

CMF C44 H44 Cu N8

CCI CCS

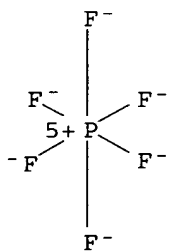


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 43 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:731813 CAPLUS

DOCUMENT NUMBER: 126:3785

TITLE: Fluorogenic β-lactam preparation and  
β-lactamase reporter gene assay for animal

cell transcription, transfection, or  
antibiotic resistance  
INVENTOR(S): Tsien, Roger Y.; Zlokarnik, Gregor  
PATENT ASSIGNEE(S): University of California, USA  
SOURCE: PCT Int. Appl., 118 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

| PATENT NO.  | KIND            | DATE     | APPLICATION NO. | DATE        |
|---|-----------------|----------|-----------------|-------------|
| WO 9630540  | A2              | 19961003 | WO 1996-US4059  | 19960320    |
| WO 9630540  | A3              | 19970109 |                 |             |
| W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI |                 |          |                 |             |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN  |                 |          |                 |             |
| US 5741657  | A               | 19980421 | US 1995-407544  | 19950320    |
| CA 2215310  | AA              | 19961003 | CA 1996-2215310 | 19960320    |
| CA 2215310  | C               | 20020521 |                 |             |
| AU 9655266  | A1              | 19961016 | AU 1996-55266   | 19960320    |
| AU 723164   | B2              | 20000817 |                 |             |
| EP 817785   | A2              | 19980114 | EP 1996-912454  | 19960320    |
| EP 817785   | B1              | 20010404 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI   |                 |          |                 |             |
| CN 1184479  | A               | 19980610 | CN 1996-193854  | 19960320    |
| CN 1066731  | B               | 20010606 |                 |             |
| JP 11502714   | T2              | 19990309 | JP 1996-529573  | 19960320    |
| JP 3633940  | B2              | 20050330 |                 |             |
| AT 200287   | E               | 20010415 | AT 1996-912454  | 19960320    |
| ES 2156994  | T3              | 20010801 | ES 1996-912454  | 19960320    |
| AT 253632   | E               | 20031115 | AT 1999-118473  | 19960320    |
| PT 982398   | T               | 20040227 | PT 1999-118473  | 19960320    |
| EP 1405922  | A2              | 20040407 | EP 2003-25361   | 19960320    |
| EP 1405922  | A3              | 20040929 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI   |                 |          |                 |             |
| ES 2209305  | T3              | 20040616 | ES 1999-118473  | 19960320    |
| US 6291162  | B1              | 20010918 | US 1996-727616  | 19961015    |
| EP 982398   | A1              | 20000301 | EP 1999-118473  | 19990917    |
| EP 982398   | B1              | 20031105 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI   |                 |          |                 |             |
| US 6472205  | B1              | 20021029 | US 2000-481756  | 20000111    |
| CN 1296078  | A               | 20010523 | CN 2000-122761  | 20000808    |
| US 2003119085   | A1              | 20030626 | US 2002-280482  | 20021024    |
| JP 2005021172   | A2              | 20050127 | JP 2004-305450  | 20041020    |
| PRIORITY APPLN. INFO.:  |                 |          | US 1995-407544  | A2 19950320 |
|   |                 |          | EP 1996-912454  | A3 19960320 |
|   |                 |          | JP 1996-529573  | A3 19960320 |
|   |                 |          | WO 1996-US4059  | W 19960320  |
|   |                 |          | US 1996-727616  | A1 19961015 |
|   |                 |          | EP 1999-118473  | A3 19990917 |
|   |                 |          | US 2000-481756  | A1 20000111 |
| OTHER SOURCE(S):  | MARPAT 126:3785 |          |                 |             |

- AB **Fluorogenic**  $\beta$ -lactam substrates are useful for detecting expression of the reporter gene,  $\beta$ -lactamase gene. Synthetic  $\beta$ -lactamase substrates with a **fluorescent** donor moiety in addition to a quencher moiety (which may or may not re-emit) are prepared and characterized. Synthetic substrates may include groups which are alkyl of 1 to about 5 carbon atoms or  $(CH_2)_nOH$ , in which n is 0 or an integer from 1 to 5. Synthetic substrates also may include physiologically acceptable metal and ammonium cations,  $-CHR_2OCO(CH_2)_nCH_3$ ,  $-CHR_2OCOC(CH_3)_3$ , acylthiomethyl, acyloxy- $\alpha$ -benzyl,  $\delta$ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulphinylmethyl,  $\beta$ -morpholinoethyl, dialkylaminoethyl, acyloxyalkyl, and dialkylaminocarbonyloxymethyl groups. S, O, SO, SO<sub>2</sub> and CH<sub>2</sub> as well as linkers for the **fluorescent** donor and quencher moieties are also included in synthetic  $\beta$ -lactamase substrates. Methods of assaying  $\beta$ -lactamase activity and monitoring expression in systems using  $\beta$ -lactamase as a reporter gene also are disclosed. Examples include Drosophila or zebrafish embryo transformation assays as well as animal **cell** glucocorticoid receptor-mediated or  $\beta$ -adrenergic receptor-mediated transcription assays.
- IC ICM C12Q
- CC 7-3 (Enzymes)
- Section cross-reference(s): 1, 3, 10, 26
- ST lactam beta **fluorescent** prep transcription assay; cephalosporin **fluorogenic** prep gene transcription assay; lactamase beta reporter gene assay **fluorescence**; transformation genetic assay **fluorescent** beta lactam; antibiotic beta lactam resistance assay **fluorescence**; Bacillus beta lactamase gene sequence Escherichia
- IT Genetic element
- RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
- (CRE (cAMP-responsive element), recombinant bacterial  $\beta$ -lactamase gene containing mammalian Kozak sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Protein sequences
- (Escherichia coli and Bacillus licheniformis  $\beta$ -lactamase derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT DNA sequences
- (Escherichia coli and Bacillus licheniformis  $\beta$ -lactamase gene derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element
- RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
- (GRE (glucocorticosteroid-responsive element); **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element
- RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
- (RNA formation factor NFAT-1-responsive element, recombinant bacterial  $\beta$ -lactamase gene containing mammalian Kozak sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter



- gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element  
 RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (SRE (serum-responsive element), recombinant bacterial  $\beta$ -lactamase gene containing mammalian Kozak sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element  
 RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (TRE (phorbol myristate acetate-responsive element), recombinant bacterial  $\beta$ -lactamase gene containing mammalian Kozak sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Antibiotic resistance  
 (assay for  $\beta$ -lactam resistance detection; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Animal **cell**  
 Transcription, genetic  
 Transformation, genetic  
 (assay of gene expression in animal **cell**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Glucocorticoid receptors  
 RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (**cell** surface; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Danio rerio  
 (embryo transfection by injection; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT **Fluorescence** quenching  
**Fluorescent** probes  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Receptors  
 RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Eukaryote (Eukaryotae)  
 (gene expression host; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT T **cell** (lymphocyte)

- (mouse expression host; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Biological transport  
(permeation, **cell** membrane-permeant and -impermeant **fluorogenic** substrates; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Promoter (genetic element)  
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
(promoter activity assay, especially c-fos and c-jun promoters; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Genetic element  
RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(ribosome-binding site, recombinant bacterial  $\beta$ -lactamase gene containing mammalian Kozak sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Animal **cell** line  
Drosophila  
(transfection; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Lactams  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
( $\beta$ -, antibiotics, **fluorogenic** derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Adrenoceptors  
RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
( $\beta$ -, **cell** surface; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Lactams  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
( $\beta$ -, **fluorogenic** derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Bacillus licheniformis  
Escherichia coli  
( $\beta$ -lactamase derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT Gene, microbial

RL: ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

( $\beta$ -lactamase reporter gene expression; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-82-5P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(CCF1, preparation,  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-52-9P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(CCF2, preparation and reaction with acetoxymethylbromide,  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-66-5P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(CCF2/ac2AM2, preparation, membrane permeable  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-69-8P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(CCF2/btAMac2, preparation, membrane permeant  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-65-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(CCFlac3, preparation and deacylation; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-62-1P

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(FCRE, preparation,  $\beta$ -lactam **fluorogenic** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

- IT 183736-59-6P  
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
 (FCRX, preparation,  $\beta$ -lactam **fluorogenic** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183870-59-9P  
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
 (RCF, preparation,  $\beta$ -lactam **fluorogenic** derivative;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183869-58-1P 183869-60-5P 183869-62-7P 183869-64-9P 183869-66-1P,  
 Lactamase,  $\beta$ - (Bacillus licheniformis)  
 RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (amino acid sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 957-68-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (conversion to mercapto-cephalosporanic acid and coupling with rhodol derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 51649-83-3, 5-Aminofluorescein  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (conversion to **mercaptofluorescein** or bromination;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 26973-80-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling by nucleophilic displacement reaction with **mercaptofluorescein**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-53-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling by nucleophilic displacement with diacetyl eosinithiol;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 120718-52-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling reaction with amine of bifunctional cephalosporin;  
**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 56040-80-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)

- (coupling reaction with coumarin or **fluorescein** derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-68-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction with **fluorescein**-cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 125440-93-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction with mercapto-cephalosporin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 68169-37-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction with thiol of bifunctional cephalosporin; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 84461-60-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(displacement reaction with cephalosporin amine bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 11111-12-9D, Cephalosporin, **fluorogenic** derivs.  
RL: ARG (Analytical reagent use); ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
(**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 81-88-9D, cephalosporin **fluorogenic** derivs. 91-64-5D, Coumarin, cephalosporin **fluorogenic** derivs. 93-35-6D, 7-Hydroxycoumarin, cephalosporin **fluorogenic** derivs. 574-93-6D, Phthalocyanine, **fluorogenic**  $\beta$ -lactam derivs. 2320-96-9D, **Dichlorofluorescein**, cephalosporin **fluorogenic** derivs. 2321-07-5D, **Fluorescein**, cephalosporin **fluorogenic** derivs. 3086-44-0D, Rhodol, cephalosporin **fluorogenic** derivs. 7440-27-9D, Terbium, **fluorogenic**  $\beta$ -lactam derivs., biological studies 7440-53-1D, Europium, **fluorogenic**  $\beta$ -lactam derivs., biological studies 17372-87-1D, Eosin, cephalosporin **fluorogenic** derivs. 26761-84-2D, **Tetrachlorofluorescein**, cephalosporin **fluorogenic** derivs. 87893-58-1D, 6-Chloro-7-hydroxycoumarin, cephalosporin **fluorogenic** derivs. 183736-85-8 183736-86-9 **183736-87-0**  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
(**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 9073-60-3P,  $\beta$ -Lactamase  
RL: ARU (Analytical role, unclassified); BAC (Biological activity or

effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183869-57-0 183869-59-2 183869-61-6 183869-63-8 183869-65-0  
RL: ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(nucleotide sequence; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 9000-82-2, Citrus acetyl esterase  
RL: CAT (Catalyst use); USES (Uses)

(orange peel; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-58-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and bromide displacement reaction with **fluoresceinthiol**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-81-4P 183736-83-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cleavage reaction; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-60-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and conversion to eosinthiol diacetate dimer; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 75900-75-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and conversion to mercapto-eosin; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-54-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling by nucleophilic displacement with cephalosporin acetate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-49-4P 183736-56-3DP, bromoacetamide derivs. 183736-78-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling reaction with cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or

- antibiotic resistance)
- IT 183743-61-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-51-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with coumarin-cephalosporanic acid derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-63-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with **fluoresceinthiol** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-80-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reaction with mercapto-**fluorescein** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 56654-74-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling reactions with **fluorescein**, rhodamine, or resorufin derivs.; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-61-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling with **fluoresceinthiol**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-79-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and conversion to iodo-derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-64-3P 183736-75-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deprotection; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-47-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with benzylglycine; **fluorogenic**

- $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-57-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromoacetyl bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-73-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromoacetyl bromide; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-84-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromomethylacetate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-74-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with butyric anhydride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 5269-39-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 131088-02-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with malonate; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-71-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with resorcinol; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 97461-45-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with silyl-sarcosine derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)
- IT 183736-76-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT



- (Reactant or reagent)  
(preparation and reduction to monomer; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-70-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction to monomers; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 183736-55-2P  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation,  $\beta$ -lactam **fluorescent** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 107-97-1, Sarcosine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with N-Me **trimethylsilyltrifluoroacetamide**; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 106-31-0, Butyric anhydride 1738-76-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with coumarin derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 140-89-6, Potassium ethylxanthate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with eosinamine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 79349-53-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with **fluorescein** derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 5466-84-2, 4-Nitrophthalic anhydride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with hydroxyjulolidine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 108-46-3, 1,3-Benzenediol, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with hydroxyjulolidine derivative; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 41175-50-2, 8-Hydroxyjulolidine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with nitrophthalic anhydride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)
- IT 24589-78-4, N-Methyl-N-(trimethylsilyl)**trifluoroacetamide**  
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with sarcosine; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-77-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with thionyl chloride; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

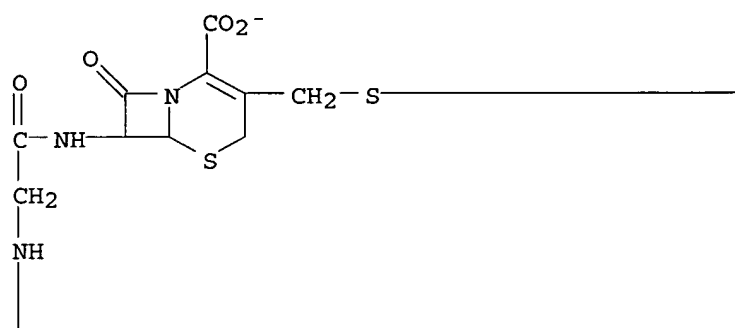
IT 95-88-5, 4-Chlororesorcinol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

IT 183736-72-3P  
 RL: BYP (Byproduct); PREP (Preparation)  
 (synthetic byproduct; **fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

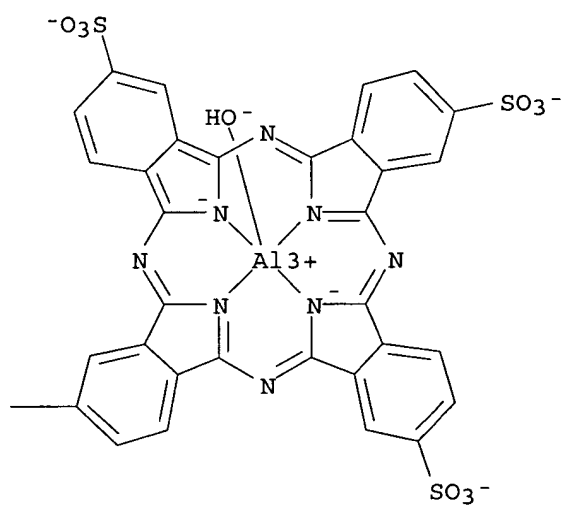
IT 183736-87-0  
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)  
 (**fluorogenic**  $\beta$ -lactam preparation and  $\beta$ -lactamase reporter gene assay for animal **cell** transcription, transfection, or antibiotic resistance)

RN 183736-87-0 CAPLUS  
 CN Europate(2-), [ $\mu$ -[10-[[[2-[[2-carboxy-8-oxo-3-[[[9,16,23-trisulfo-29H,31H-phthalocyanin-2-yl)thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl]amino]-2-oxoethyl]amino]carbonyl]-1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5-carboxylato(8-)-N1,N14,N39,N40,N41,N42,N43,N44:N29,N30,N31,N32]](hydroxyaluminate)-(9CI) (CA INDEX NAME)

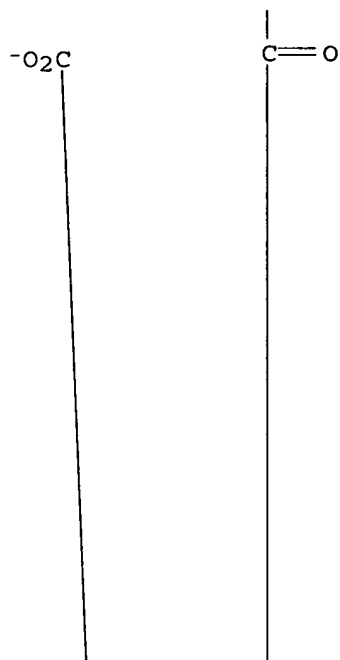
PAGE 1-A



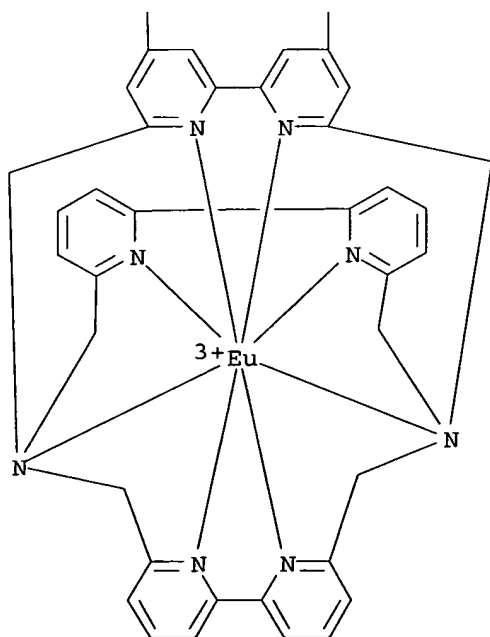
PAGE 1-B



PAGE 2-A



PAGE 3-A



L79 ANSWER 44 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1996:710159 CAPLUS  
 DOCUMENT NUMBER: 126:16172

TITLE: Structure and Reactivity of a Dinuclear Cobalt(III) Complex with a Bridging **Phosphate** Monoester

AUTHOR(S): Seo, Jin Seog; Sung, Nack-Do; Hynes, Rosemary C.; Chin, Jik

CORPORATE SOURCE: Department of Chemistry, McGill University, Montreal, QC, H3A 2K6, Can.

SOURCE: Inorganic Chemistry (1996), 35(26), 7472-7473  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The **phosphate** monoester in [Co<sub>2</sub>(bpmp)(O<sub>3</sub>P(OPh))(OH<sub>2</sub>)(OH)](ClO<sub>4</sub>)<sub>2</sub> (2, where bpmp is the phenoxy anion form of 2,6-bis(bis(2-pyridylmethyl)aminomethyl)-4-methylphenol) is hydrolyzed an unprecedented 1011-fold more rapidly than the corresponding unbound **phosphate**. Clean cleavage of the bidentate monoester, together with the crystal structure of [Co<sub>2</sub>(bpmp)(O<sub>3</sub>P(Ph))(OH<sub>2</sub>)(OH)](ClO<sub>4</sub>)<sub>2</sub> (1) provide detailed mechanistic insight into the hydrolysis reaction.

CC 7-4 (Enzymes)  
Section cross-reference(s): 67, 75, 78

ST dinuclear cobalt complex prepn **phosphomonoesterase** model; **phosphatase** model dinuclear cobalt complex prepn; crystal structure dinuclear cobalt complex

IT Enzyme functional sites  
(active, model; preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT Complexation  
(of cobalt; preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT Crystal structure  
Hydrolysis kinetics  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT 7440-48-4, Cobalt, properties  
RL: PRP (Properties)  
(coordination; preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT 9013-05-2, **Phosphomonoesterase**  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT 184358-73-4P  
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT 184358-71-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with a bridging **phosphate** monoester as a **phosphomonoesterase** model)

IT 701-64-4, Phenyl **phosphate** 13455-31-7, Cobalt diperchlorate 25148-85-0, Disodium **phenylphosphonate** 80528-41-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with  
a bridging **phosphate** monoester as a  
**phosphomonoesterase** model)

IT 184358-73-4P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation, structure, and reactivity of a dinuclear Co(III) complex with  
a bridging **phosphate** monoester as a  
**phosphomonoesterase** model)

RN 184358-73-4 CAPLUS

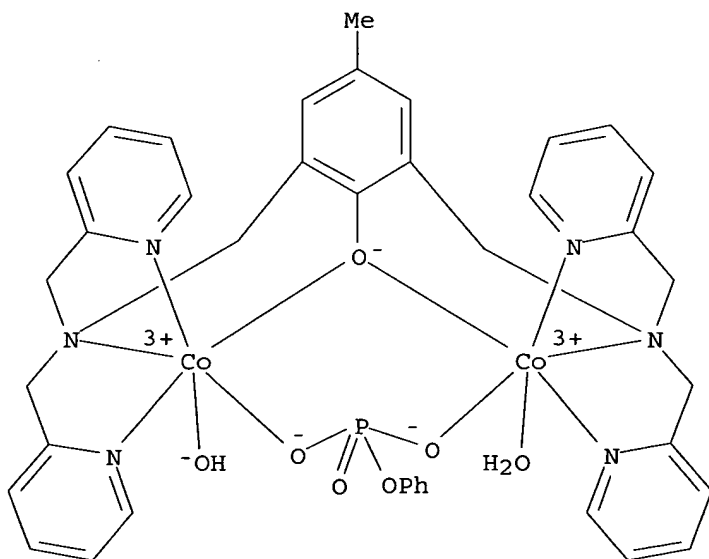
CN Cobalt(2+), aqua [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]methyl]-4-methylphenolato- $\kappa$ O: $\kappa$ O]]hydroxy [ $\mu$ -  
[monophenyl phosphato(2-)- $\kappa$ O': $\kappa$ O'']]di-, diperchlorate (9CI)  
(CA INDEX NAME)

CM 1

CRN 184358-72-3

CMF C39 H41 Co2 N6 O7 P

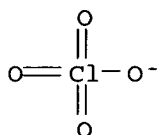
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 184358-71-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, structure, and reactivity of a dinuclear Co(III) complex with  
 a bridging phosphate monoester as a  
 phosphomonoesterase model)

RN 184358-71-2 CAPLUS

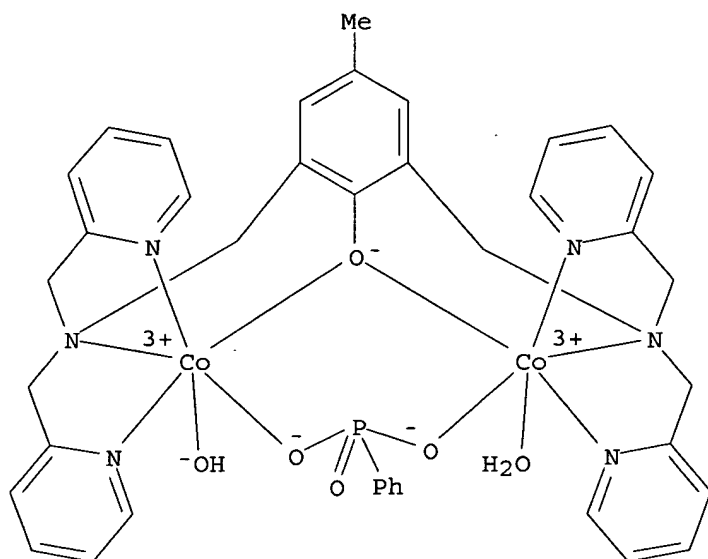
CN Cobalt(2+), aqua [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]methyl]-4-methylphenolato- $\kappa$ O: $\kappa$ O]]hydroxy[ $\mu$ -[phenylphosphonato(2-)- $\kappa$ O: $\kappa$ O']]di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 184358-70-1

CMF C39 H41 Co2 N6 O6 P

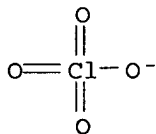
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 45 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

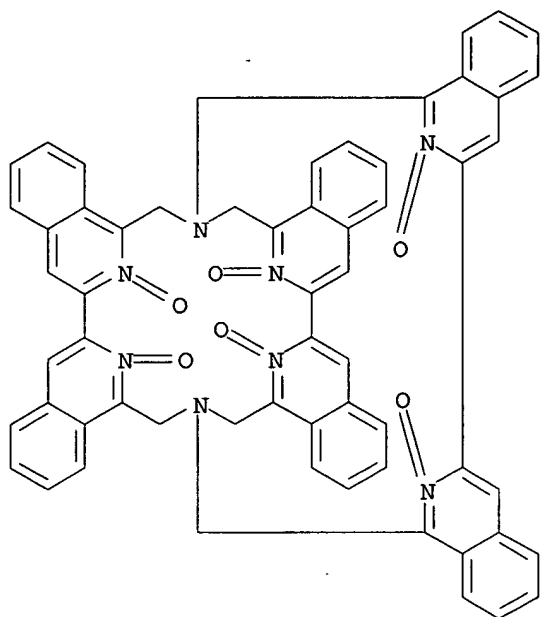
ACCESSION NUMBER: 1996 559605 CAPLUS

DOCUMENT NUMBER: 125:311363

TITLE: Luminescent macrocyclic lanthanide complexes bearing

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L79 ANSWER 46 OF 52 CAPLUS, COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:961617 CAPLUS

DOCUMENT NUMBER: 124:98952

TITLE: Reversible O<sub>2</sub> Binding to a Dinuclear Copper(I) Complex with Linked Tris(2-pyridylmethyl)amine Units: Kinetic-Thermodynamic Comparisons with Mononuclear Analogs

AUTHOR(S): Lee, Dong-Heon; Wei, Ning; Murthy, Narasimha N.; Tyeklar, Zoltan; Karlin, Kenneth D.; Kaderli, Susan; Jung, Bernhard; Zuberbuehler, Andreas D.

CORPORATE SOURCE: Department of Chemistry, Johns Hopkins University, Baltimore, MD, 21218, USA

SOURCE: Journal of the American Chemical Society (1995), 117(50), 12498-513

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The kinetics and thermodyn. of reaction of O<sub>2</sub> with copper(I) complexes can provide fundamental information relevant to chemical and biol. systems. Using diode-array variable-temperature (180-296 K) stopped-flow kinetic methods,

we report detailed information on the O<sub>2</sub> reactivity (in EtCN) of dicopper(I) complex [(D1)CuI<sub>2</sub>(RCN)<sub>2</sub>]<sub>2</sub><sup>2+</sup> (2a) (R = Me or Et) [D1 = dinucleating ligand with a -CH<sub>2</sub>CH<sub>2</sub>- group linking two tris(2-pyridylmethyl)amine (TPMA) units at a 5-pyridyl position of each tetradentate moiety]. A comparative study of mononuclear complex [(TMPAE)Cu(RCN)]<sup>+</sup> (1a') [TMPAE has a -C(O)OCH<sub>3</sub> ester substituent in the 5-position of one pyridyl group of TPMA] has been carried out. The results are compared with data from the previously investigated complex [(TPMA)Cu(RCN)]<sup>+</sup> (1a). The syntheses of D1 and 2a-(ClO<sub>4</sub>)<sub>2</sub> are described; an x-ray structure reveals two pentacoordinate Cu(I) ions (Cu...Cu = 11.70 Å), each bound by the N<sub>4</sub>-tetradentate and an EtCN mol. Cyclic voltammetric data for a' and a

are reported. At 193 K in EtCN, a reacts with O<sub>2</sub> (Cu/O<sub>2</sub> = 2:1, manometry) to produce an intensely purple colored solution of adduct [(D1)Cu<sub>2</sub>(O<sub>2</sub>)]<sub>2</sub><sup>+</sup> (c), λ<sub>max</sub> = 540 nm (ε = 11,100 M<sup>-1</sup> cm<sup>-1</sup>). This peroxo-dicopper(II) species reacts with PPh<sub>3</sub>, liberating O<sub>2</sub> and producing the isolatable bis-phosphine adduct [(D1)Cu<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup>. The kinetic investigation provides spectral characterization of transient Cu/O<sub>2</sub> 1:1 adducts generated upon oxygenation of cold solns. of a' or a. [(TMPAE)Cu(O<sub>2</sub>)]<sup>+</sup> (b') forms reversibly (λ<sub>max</sub> = 415 nm) with k<sub>1</sub> = (8.2 ± 0.4) + 103 M<sup>-1</sup> s<sup>-1</sup> and K<sub>1</sub> = k<sub>1</sub>/k<sub>-1</sub> = (284 ± 9) M<sup>-1</sup> at 183 K, with ΔH<sub>1</sub><sup>°</sup> = (-32 ± 1) kJ mol<sup>-1</sup>, ΔS<sub>1</sub><sup>°</sup> = (-127 ± 3) J K<sup>-1</sup> mol<sup>-1</sup>. Two types of Cu(II)-O<sub>2</sub>- complexes form in the reaction of a: a 2:1 open form (i.e., [(D1)Cu<sub>2</sub>(O<sub>2</sub>)(EtCN)]<sub>2</sub><sup>+</sup>, 2b) and a bis-O<sub>2</sub> 2:2 open adduct (i.e., [(D1)Cu<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup>, 2b'). For the formation of 2b, k<sub>1</sub> = (1.63 ± 0.01) + 104 M<sup>-1</sup> s<sup>-1</sup> and K<sub>1</sub> = (2.03 ± 0.04) + 103 M<sup>-1</sup> at 183 K. Complexes 2b and 2b' have identical spectroscopic properties (λ<sub>max</sub> = 416 nm), ε = 4500 M<sup>-1</sup> cm<sup>-1</sup> per Cu-O<sub>2</sub> unit, and their rate consts. are statistically related. Intermediates 1b' and 2b further convert into (μ-peroxo)dicopper(II) [(2 Cu):(1 O<sub>2</sub>)] complexes. [{(TMPAE)Cu}<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup> (1c') (λ<sub>max</sub> = 532 nm, ε = 9380 M<sup>-1</sup> cm<sup>-1</sup>) forms in a second-order reaction of 1b' with 1a' with K<sub>1</sub>K<sub>2</sub> = (2.1 ± 0.4) + 1011 M<sup>-2</sup> at 183 K (ΔH<sub>12</sub><sup>°</sup> = -77 ± 1 kJ mol<sup>-1</sup> and ΔS<sub>12</sub><sup>°</sup> = -203 ± 5 J K<sup>-1</sup> mol<sup>-1</sup>), while [(D1)Cu<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup> (2c) (λ<sub>max</sub> = 540, ε 11 100 M<sup>-1</sup> cm<sup>-1</sup>) is generated from 2b in an intramol. reaction, with k<sub>2</sub> = (3.51 ± 0.05) + 101 s<sup>-1</sup> and k<sub>on</sub> = k<sub>1</sub>k<sub>2</sub>/k<sub>-1</sub> = (7.1 ± 0.2) + 104 M<sup>-1</sup> s<sup>-1</sup> (183 K). The overall formation of 2c is faster than for 1c' or [{(TMPA)Cu}<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup> (1c) because of a more pos. entropy of activation (ΔS<sub>on.thermod.</sub> = (-139 ± 3) J K<sup>-1</sup> mol<sup>-1</sup> for 2c vs ΔS<sub>on.thermod.</sub> = (-201 ± 5) J K<sup>-1</sup> mol<sup>-1</sup> for 1c). However, this significantly enhanced kinetic reactivity (for 2a → 2c) is not reflected by an analogous increase in thermodyn. stability. [(D1)Cu<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>]<sub>2</sub><sup>+</sup> (2c) is enthalpically less stable (ΔH<sub>12</sub><sup>°</sup> = (-34.8 ± 0.4) kJ mol<sup>-1</sup>) than Cu<sub>2</sub>O<sub>2</sub> species 1c and 1c' (ΔH<sub>12</sub><sup>°</sup> = -81 to -77 kJ mol<sup>-1</sup>, resp.), which are formed from mononuclear precursors. There is a substantially larger overall formation entropy for 2c [ΔS<sub>12</sub><sup>°</sup> = (-89.3 ± 1.5) J K<sup>-1</sup> mol<sup>-1</sup> compared to -220 and -203 J K<sup>-1</sup> mol<sup>-1</sup> for 1c and 1c', resp.] since Cu<sub>2</sub>O<sub>2</sub> formation is an intramol., rather than intermol., process. Examination of other kinetic parameters and spectral differences provides complementary information that 2c has a strained structure. In fact, 2c is not the ultimate oxidation product: relief of steric constraints occurs at higher temps. by a slow rearrangement (λ<sub>max</sub> = 540 nm → λ<sub>max</sub> = 529 nm) producing {Cu<sub>2</sub>O<sub>2</sub>}<sub>n</sub> oligomers containing intermol. Cu-O<sub>2</sub>-Cu bonds. A particularly stable trimer species [{(D1)Cu<sub>2</sub>(O<sub>2</sub>)<sub>2</sub>}]<sub>3</sub><sup>6+</sup> (2d) was characterized, with ΔH<sub>3</sub><sup>°</sup> = (-153 kJ mol<sup>-1</sup>)/3 = -51 kJ mol<sup>-1</sup> per Cu<sub>2</sub>O<sub>2</sub> unit, intermediate between that seen for 2c, 1c, and 1c'. Thus, (peroxo)dicopper(II) complexes formed from mononuclear precursors are the most stable, while secondary rearrangements within intramolecularly formed Cu<sub>2</sub>-O<sub>2</sub> complexes with dinucleating ligands can and do occur. Comparisons are made with relevant copper-dioxygen complexes, and the chemical and biol. relevance of this chemical is discussed.

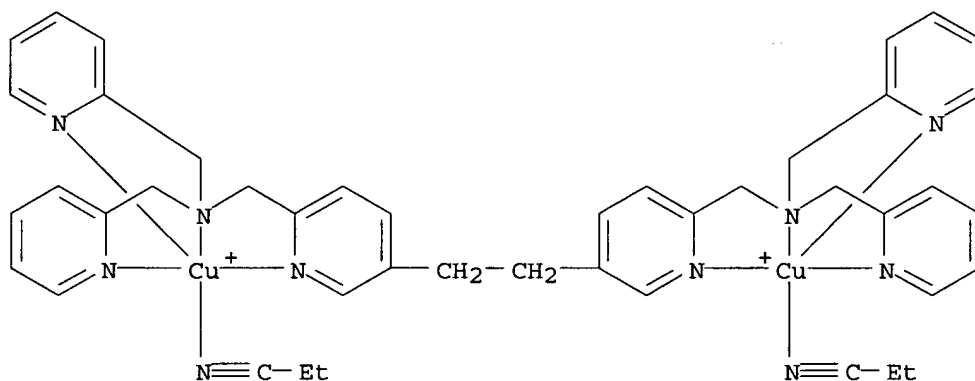
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)  
Section cross-reference(s): 69, 78

IT 603-35-0, **Triphenylphosphine**, reactions 7782-44-7, Oxygen,  
reactions 147186-21-8 **157958-87-7** **172696-96-7**

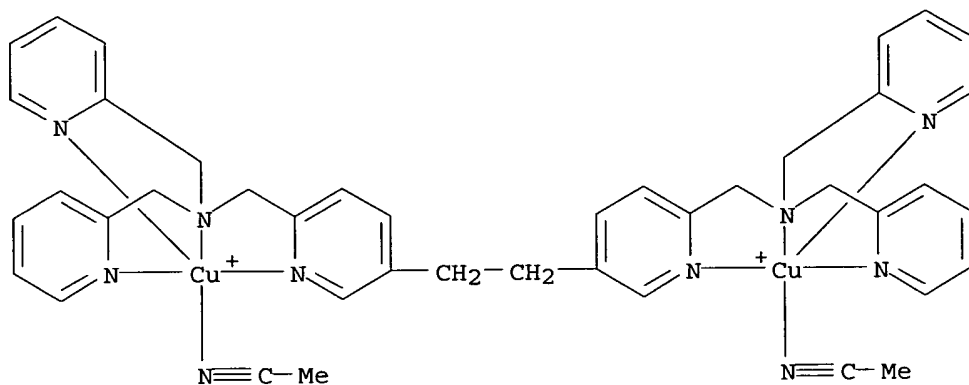
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)

- IT 157958-88-8P 157997-68-7P 172696-99-0P 172807-44-2P  
172807-45-3P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)
- IT 7440-50-8DP, Copper, pyridylmethylamine oxygen trimer complex  
7782-44-7DP, Oxygen, copper pyridylmethylamine trimer complex  
157958-89-9P 172696-97-8P 172696-98-9P  
172696-99-0DP, copper oxygen trimer complex  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)
- IT 157958-87-7 172696-96-7  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)
- RN 157958-87-7 CAPLUS  
CN Copper(2+), [μ-[5,5'-(1,2-ethanediyl)bis[N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]]bis(propanetriole)di- (9CI) (CA INDEX NAME)



- RN 172696-96-7 CAPLUS  
CN Copper(2+), bis(acetonitrile) [μ-[5,5'-(1,2-ethanediyl)bis[N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]]]di- (9CI) (CA INDEX NAME)



IT 157958-88-8P 157997-68-7P 172807-45-3P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)

RN 157958-88-8 CAPLUS

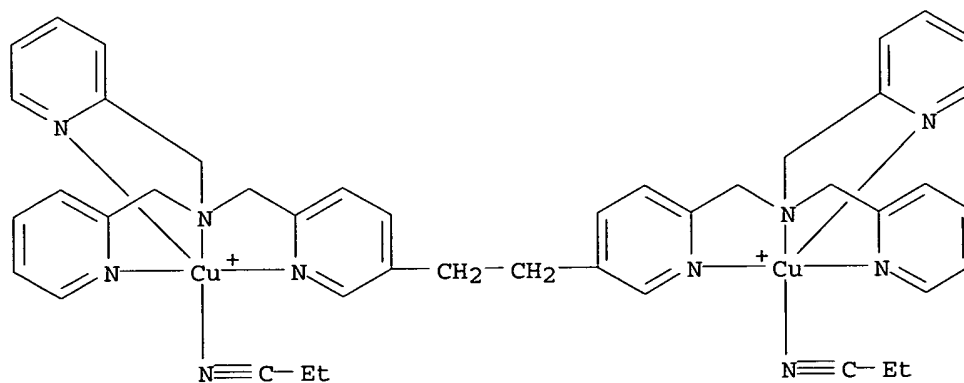
CN Copper(2+), bis(acetonitrile) [ $\mu$ -[5,5'-(1,2-ethanediyl)bis[N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]]]di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 157958-87-7

CMF C44 H48 Cu2 N10

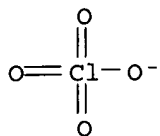
CCI CCS



CM 2

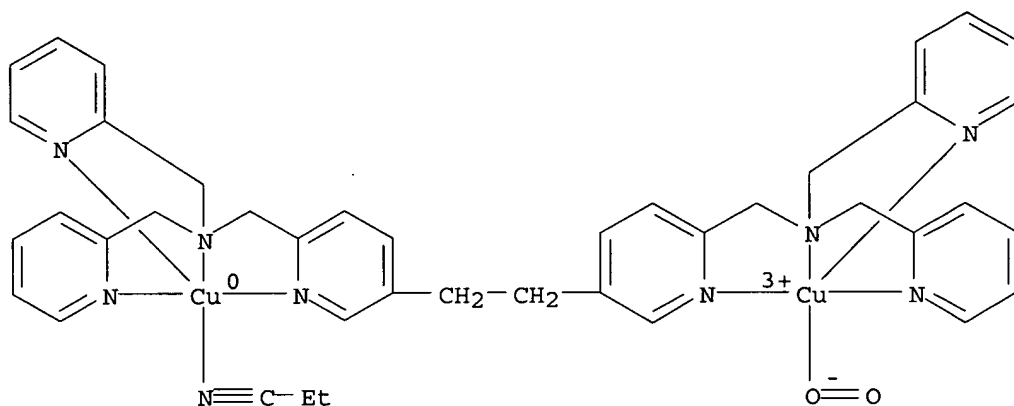
CRN 14797-73-0

CMF Cl O4



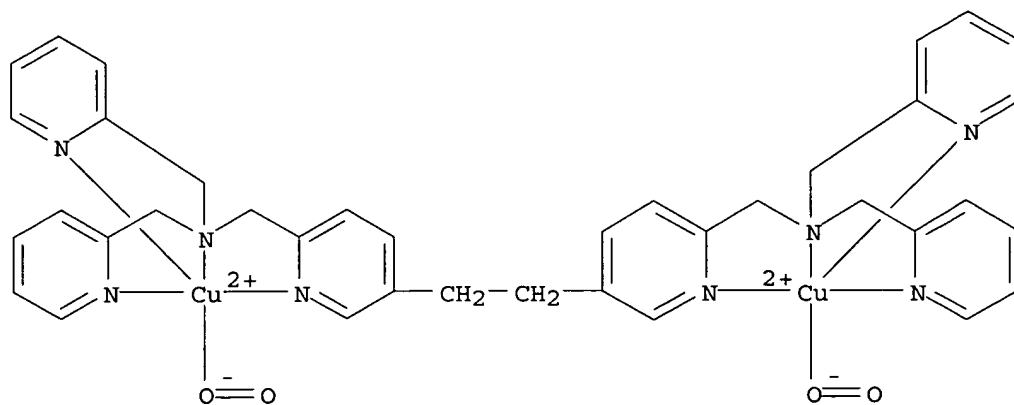
RN 157997-68-7 CAPLUS

CN Copper (2+), [μ-[5,5'-(1,2-ethanediyl)bis[N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]]](propanenitri  
le)superoxidodi- (9CI) (CA INDEX NAME)



RN 172807-45-3 CAPLUS

CN Copper, [μ-[5,5'-(1,2-ethanediyl)bis[N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]]]disuperoxidod  
i- (9CI) (CA INDEX NAME)



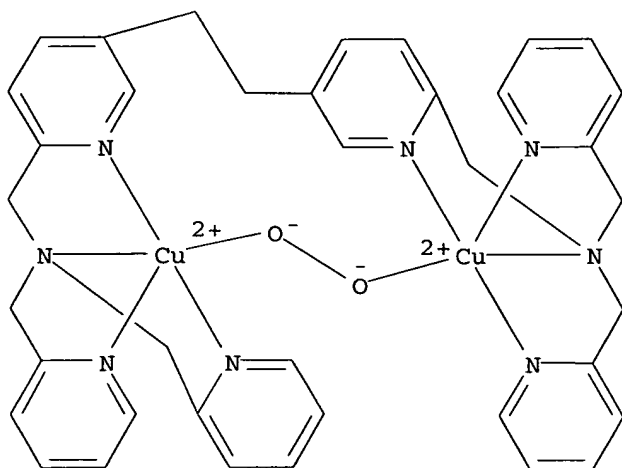
IT 157958-89-9P 172696-97-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(reversible O<sub>2</sub> binding to dinuclear copper(I) complex with linked tris(2-pyridylmethyl)amine units and kinetic-thermodn. comparisons with mononuclear analogs)

RN 157958-89-9 CAPLUS

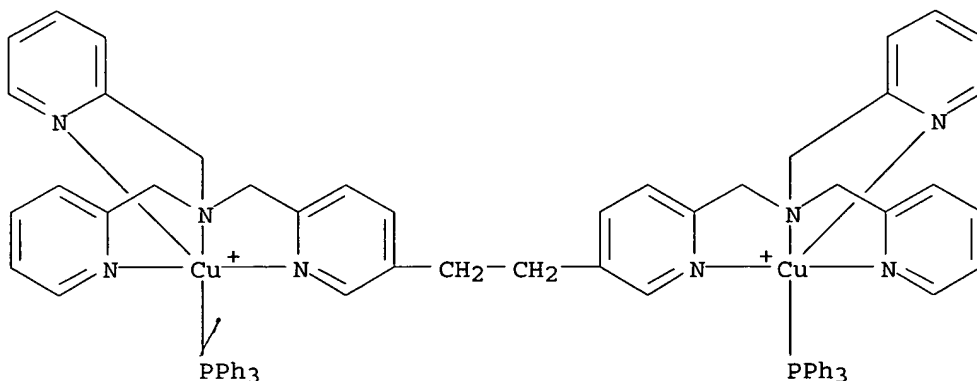
CN Copper (2+), [μ-[5,5'-(1,2-ethanediyl)bis[N,N-bis[(2-pyridinyl-

$\kappa N$  methyl]-2-pyridinemethanamine- $\kappa N1, \kappa N2$ ]] [ $\mu$ -(peroxy- $\kappa O: \kappa O'$ )]di- (9CI) (CA INDEX NAME)



RN 172696-97-8 CAPLUS

CN Copper(2+), [ $\mu$ -[5,5'-(1,2-ethanediyl)bis[N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]]]bis(triphenylphosphine)di- (9CI) (CA INDEX NAME)



L79 ANSWER 47 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:413201 CAPLUS

DOCUMENT NUMBER: 123:78355

TITLE: XAS Investigations on the Iron-Zinc Center of Purple Acid Phosphatase from Red Kidney Beans  
 AUTHOR(S): Priggemeyer, S.; Eggers-Borkenstein, P.; Ahlers, F.; Krebs, B.; Henkel, G.; Koerner, M.; Witzel, H.; Nolting, H.-F.; Hermes, C.

CORPORATE SOURCE: Anorganisch-Chemisches Institut, Universitaet Muenster, Muenster, 48149, Germany

SOURCE: Inorganic Chemistry (1995), 34(6), 1445-54

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB X-ray absorption measurements are used to study the iron-zinc center of purple acid **phosphatase** isolated from red kidney beans. XANES and EXAFS data were taken at the iron and the zinc K-edge of the native enzyme (pH 7) and of the enzyme after addition of **phosphate** at pH 7 and pH 4. In the native enzyme both the iron and zinc ions are coordinated by five O/N donor ligands. The first shell EXAFS data yield a model with 2.4 O/N at 1.91 Å + 2.6 N/O at 2.10 Å around the iron atom, and 3.4 N/O at 1.97 Å + 1.6 N/O at 2.08 Å around the zinc atom. An iron-zinc distance of 3.96 Å was determined. No evidence for a bridging oxo group (indicated by doxo ca. 1.8 Å) could be obtained. After addition of **phosphate** the iron edge shifts to lower and the Zn edge to higher energies. At pH 7 the coordination nos. of iron and zinc increase to six (2.4 N/O at 1.94 Å + 3.6 N/O at 2.12 Å, Fe K-edge, and 4.0 N/O at 1.98 Å + 2.0 N/O at 2.11 Å, Zn K-edge). Since the iron-zinc distance decreases by 0.28 Å to 3.68 Å we propose a bridging coordination mode of **phosphate** at pH 7. Lowering the pH value to 4 does not affect the binding of **phosphate**. The features of the higher shell peaks in the Fourier transformed spectra remain essentially unchanged and the iron-zinc distance is maintained ( $d(\text{Fe-Zn}) = 3.69 \text{ Å}$ ). The ligand atoms in the first shells, however, are more disordered, indicating the involvement of protonation equilibrium in the first coordination spheres (2.8 N/O at 1.97 Å and 3.2 N/O at 2.19 Å, Fe K-edge, and 4.7 N/O at 2.05 Å and 1.3 N/O at 2.18 Å, Zn K-edge). These results are checked against structural data from XAS and crystallog. studies of a number of iron and zinc model complexes with mixed ligand environments and structural characteristics similar to those expected for the enzyme samples.

CC 7-5 (Enzymes)

ST purple acid **phosphatase** iron zinc site

IT Enzyme functional sites  
(XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT Coordination  
(of iron and zinc; XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT Bean  
(kidney, XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT 9001-77-8  
RL: PRP (Properties)  
(XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT 7439-89-6, Iron, properties 7440-66-6, Zinc, properties  
RL: PRP (Properties)  
(coordination; XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT 14265-44-2, **Phosphate**, miscellaneous  
RL: MSC (Miscellaneous)  
(effect on iron and zinc coordination; XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT 15308-73-3 74194-01-7 113056-40-9 115226-68-1  
126875-98-7 162338-76-3 162902-07-0 164802-63-5  
RL: PRP (Properties)  
(models; XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

IT 113056-40-9 126875-98-7  
RL: PRP (Properties)  
(models; XAS investigations on iron-zinc center of purple acid **phosphatase** from red kidney beans)

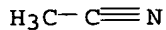
RN 113056-40-9 CAPLUS

CN Iron(2+), bis[μ-(acetato-O:O')] [μ-[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]] (zinc)-, bis[tetraphenylborate(1-)], compd. with acetonitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 113056-27-2

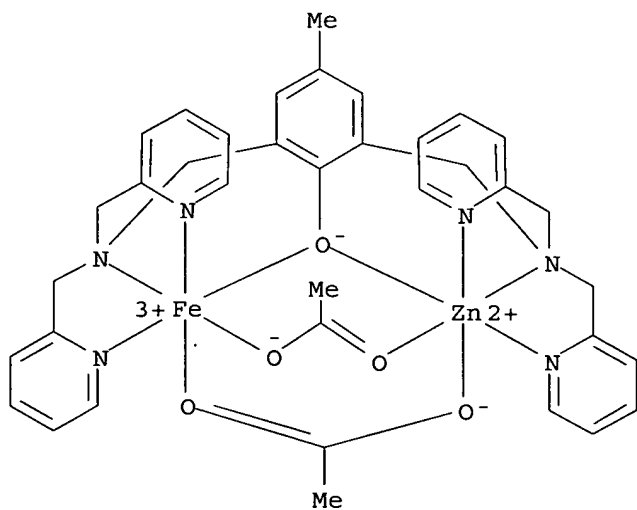
CMF C37 H39 Fe N6 O5 Zn . 2 C24 H20 B

CM 3

CRN 113056-26-1

CMF C37 H39 Fe N6 O5 Zn

CCI CCS



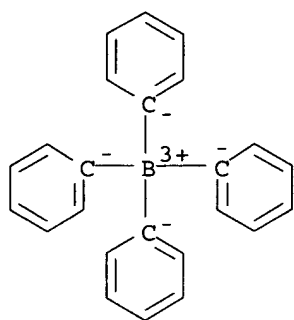
CM 4

CRN 4358-26-3

CMF C24 H20 B

CCI CCS





RN 126875-98-7 CAPLUS  
 CN Iron(2+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(diphenyl phosphato-O':O'')] (zinc)-, dperchlorate, compd. with methanol (2:3), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1

CMF C H4 O

H<sub>3</sub>C-OH

CM 2

CRN 126875-97-6

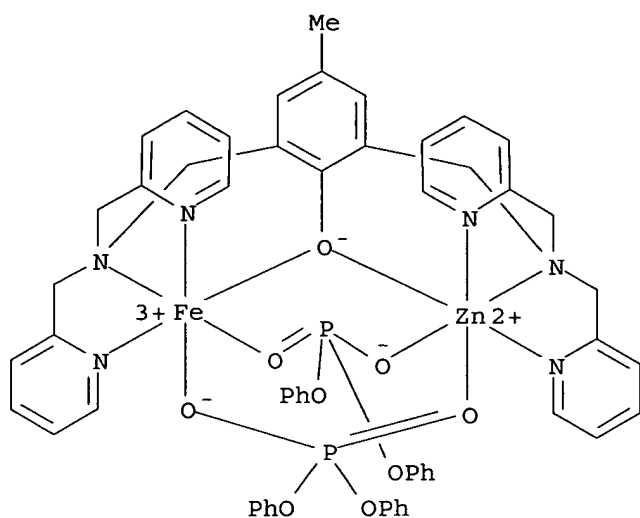
CMF C57 H53 Fe N6 O9 P2 Zn . 2 Cl O4

CM 3

CRN 126875-96-5

CMF C57 H53 Fe N6 O9 P2 Zn

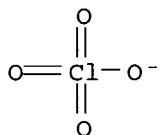
CCI CCS



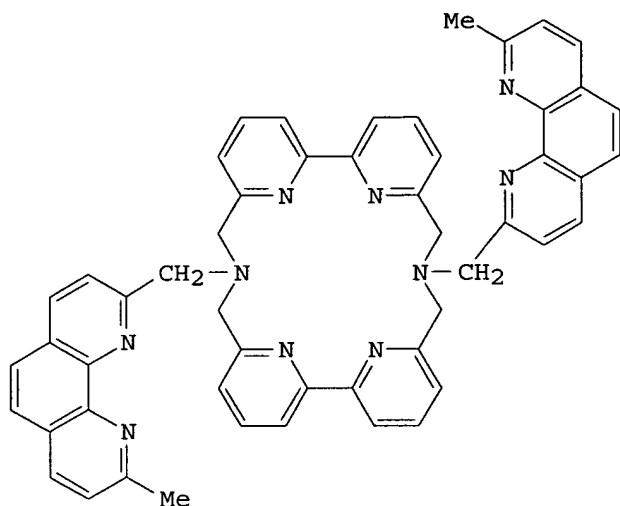
CM 4

CRN 14797-73-0

CMF Cl O4



L79 ANSWER 48 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1994:152232 CAPLUS  
 DOCUMENT NUMBER: 120:152232  
 TITLE: Synthesis and Luminescence of Lanthanide Complexes of  
 a Branched Macrocyclic Ligand Containing  
 2,2'-Bipyridine and 9-Methyl-1,10-phenanthroline  
 Subunits  
 AUTHOR(S): Sabbatini, Nanda; Guardigli, Massimo; Manet, Ilse;  
 Bolletta, Fabrizio; Ziessel, Raymond  
 CORPORATE SOURCE: Dipartimento di Chimica G. Ciamician, Universita di  
 Bologna, Bologna, 40126, Italy  
 SOURCE: Inorganic Chemistry (1994), 33(5), 955-9  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



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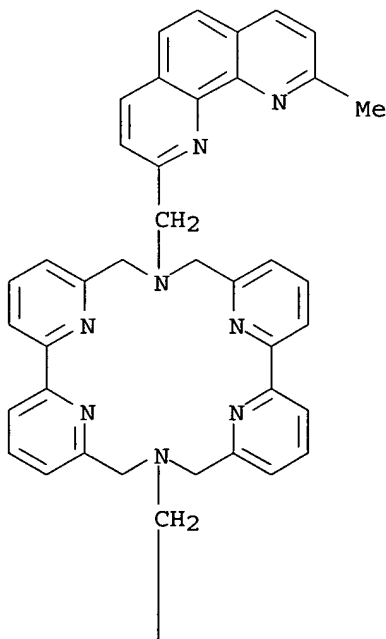
AB The synthesis of the branched-macrocyclic ligand I incorporating two 2,2'-bipyridine units in the macrocycle and two 9-methyl-1,10-phenanthroline units in the branches is described as well as the synthesis and the photophys. properties of its  $\text{Eu}^{3+}$ ,  $\text{Tb}^{3+}$ , and  $\text{Gd}^{3+}$  complexes. These complexes do not decompose in  $\text{H}_2\text{O}$  in contrast to those of the related ligand containing 2,2'-bipyridine instead of 1,10-phenanthroline. They show intense absorption bands in the UV region due to absorption in the ligand. The emission spectra of the  $[\text{EuI}]^{3+}$  and  $[\text{TbI}]^{3+}$  complexes obtained upon ligand excitation show the usual  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  transitions. The pattern of the emission spectrum of the  $[\text{EuI}]^{3+}$  complex allows the authors to assess a low (presumably C2) symmetry as the probable site symmetry of the metal ion in the complex. For  $[\text{EuI}]^{3+}$  and  $[\text{TbI}]^{3+}$ , the metal luminescence excitation spectra in  $\text{H}_2\text{O}$  match the ligand absorption spectra while in  $\text{MeOH}$  the absorption due to the phenanthroline is missing. Probably in  $\text{H}_2\text{O}$  the efficiency of the ligand-to-metal energy transfer is similar for the 2 chromophores while in  $\text{MeOH}$  phenanthroline transfers energy to the metal ion less efficiently than bipyridine. The luminescence quantum yield values in  $\text{H}_2\text{O}$  and  $\text{MeOH}$  confirm this interpretation. The lifetimes of the  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  emitting states indicate that the shielding of the metal ion from solvent mols. is rather inefficient. For the  $[\text{TbI}]^{3+}$  complex the lifetimes are temperature dependent which is attributed to the presence of an equilibrium between

the metal emitting state and triplet excited states of the ligand; this process is most likely responsible for the low luminescence quantum yields and the O effect on the  $\text{Tb}^{3+}$  luminescence. A detailed comparison between the photophys. properties in  $\text{H}_2\text{O}$  and  $\text{MeOH}$  allows the authors to conclude that the ligand I coordinates better to the metal ion in  $\text{H}_2\text{O}$  than in  $\text{MeOH}$  because of a stronger interaction in  $\text{H}_2\text{O}$  between the phenanthroline branches and the metal ion. As to the application in **fluoroimmunoassay**, the  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  complexes of the ligand I present the highest molar absorptivities among the  $\text{H}_2\text{O}$ -stable lanthanide complexes studied. The value of the incident light-emitted light conversion efficiency, obtained from the absorption and emission efficiencies, makes the  $[\text{EuI}]^{3+}$  complex interesting as a luminescent label.

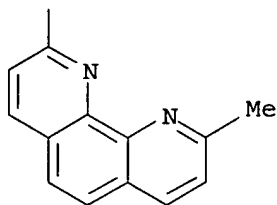
CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 9, 73

- IT **Phosphorescence**  
(of bis(phenanthrolinylmethyl)hexaazapentacyclotriacontadodecaene and its gadolinium complex)
- IT 484-11-7, 2,9-Dimethyl-1,10-phenanthroline 4411-80-7,  
6,6'-Dimethyl-2,2'-bipyridine  
RL: PRP (Properties)  
(**phosphorescence** of)
- IT 7440-27-9DP, Terbium, bis(phenanthrolinylmethyl)hexaazapentacyclotriacontadodecaene 7440-53-1DP, Europium, bis(phenanthrolinylmethyl)hexaazapentacyclotriacontadodecaene **149558-70-3DP**, europium, gadolinium and terbium complexes  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and luminescence of, in methanol and water)
- IT **149558-70-3P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and **phosphorescence** and reaction of, with lanthanide chlorides)
- IT 7440-54-2DP, Gadolinium, bis(phenanthrolinylmethyl)hexaazapentacyclotriacontadodecaene  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and **phosphorescence** of, in methanol and water)
- IT **149558-70-3DP**, europium, gadolinium and terbium complexes  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and luminescence of, in methanol and water)
- RN 149558-70-3 CAPLUS
- CN 8,21,27,28,29,30-Hexaazapentacyclo[21.3.1.12,6.110,14.115,19]triacontadodecaene,  
1(27),2,4,6(30),10,12,14(29),15,17,19(28),23,25-dodecaene,  
8,21-bis[(9-methyl-1,10-phenanthrolin-2-yl)methyl]- (9CI) (CA INDEX NAME)

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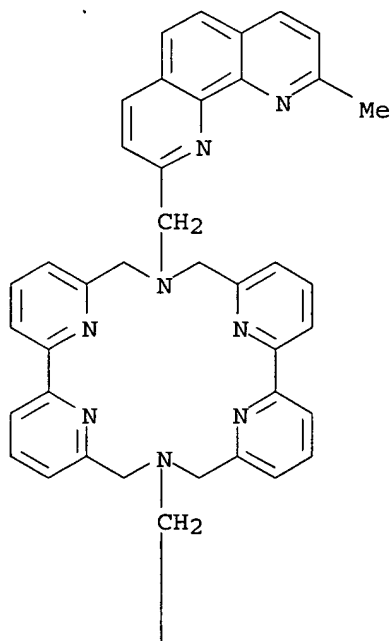
IT 149558-70-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and **phosphorescence** and reaction of, with lanthanide  
chlorides)

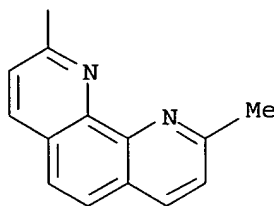
RN 149558-70-3 CAPLUS

CN 8,21,27,28,29,30-Hexaazapentacyclo[21.3.1.12,6.110,14.115,19]triaconta-  
1(27),2,4,6(30),10,12,14(29),15,17,19(28),23,25-dodecaene,  
8,21-bis[(9-methyl-1,10-phenanthrolin-2-yl)methyl]- (9CI) (CA INDEX NAME)

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L79 ANSWER 49 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:201160 CAPLUS

DOCUMENT NUMBER: 118:201160

TITLE: Reducing supermolecules to "pseudo-atoms" and anions: cryptatium species and fullerene C60

AUTHOR(S): Echegoyen, Luis; Xie, Qingshan; Perez-Cordero, Eduardo

CORPORATE SOURCE: Dep. Chem., Univ. Miami, Coral Gables, FL, 33124, USA

SOURCE: Pure and Applied Chemistry (1993), 65(3), 441-6

CODEN: PACHAS; ISSN: 0033-4545

DOCUMENT TYPE: Journal

LANGUAGE: English

AB As part of the continued interest in the redox properties of macrocyclic and macrobicyclic ligands and their corresponding metal cation complexes, the authors have recorded the electrochem. of several cryptands and their cryptates, along with those for the C clusters C60 and C70. The electrochem. of C60 and C70 at low temperature has yielded the 1st observation of the corresponding hexaanionic forms, C606- and C706-. These multiple redns. appear to be chemical and electrochem. reversible under the conditions used, so the method was employed to generate and detect C602- by ESR spectroscopy. The cryptands and cryptates studied also exhibit multiple ligand-based redox processes and, in some cases, the reduction products are isolated as crystalline materials. On a closely related topic, formation of a novel crystalline material from the reductive electrocrystn. of [Ru(bpy)3]Cl2 is reported here. The latter material is assumed to be [Ru(bpy)3]3+.

CC 72-2 (Electrochemistry)

Section cross-reference(s): 78

IT 14323-06-9, Tris(2,2'-bipyridine)ruthenium dichloride

RL: PRP (Properties)

(electrocrystn. of crystals of, in acetonitrile with tetrabutylammonium hexafluorophosphate)

IT 3109-63-5, Tetrabutylammonium hexafluorophosphate

RL: PRP (Properties)

(electrocrystn. of trisbipyridine ruthenium dichloride in acetonitrile containing)

IT 113597-85-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(redox reactions of, electrochem., in DMF on glassy carbon electrode)

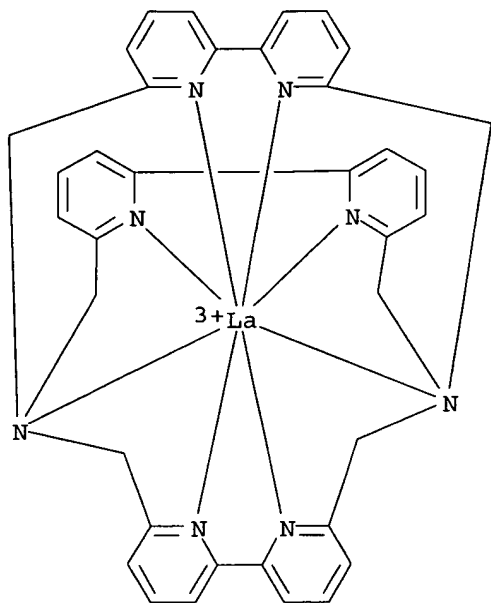
IT 113597-85-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(redox reactions of, electrochem., in DMF on glassy carbon electrode)

RN 113597-85-6 CAPLUS

CN Lanthanum(3+), (1,14,39,40,41,42,43,44-octaazaocatacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-N1,N14,N39,N40,N41,N42,N43,N44)-, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



L79 ANSWER 50 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:182105 CAPLUS

DOCUMENT NUMBER: 118:182105

TITLE: Insight into the  $g \approx 16$  EPR signals of reduced diiron-oxo proteins. Structure and properties of  $[\text{FeII}_2\text{BPMP}\{\text{O}_2\text{P}(\text{OC}_6\text{H}_5)_2\}_2]\text{Cl}$

AUTHOR(S): Jang, Ho G.; Hendrich, Michael P.; Que, Lawrence, Jr.  
CORPORATE SOURCE: Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA

SOURCE: Inorganic Chemistry (1993), 32(6), 911-18  
CODEN: INOCAJ; ISSN: 0020-1669

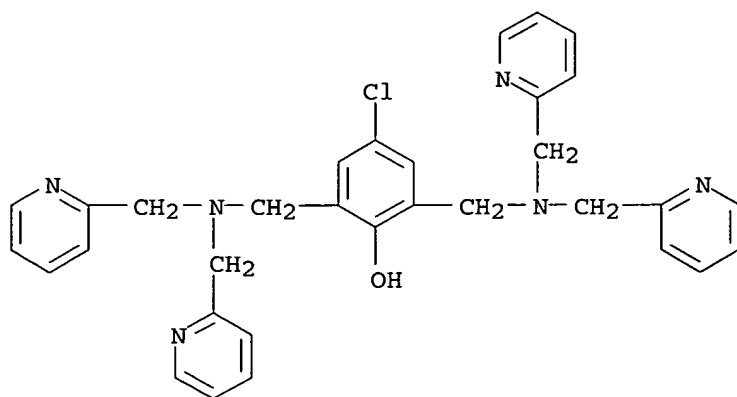
DOCUMENT TYPE: Journal

LANGUAGE: English

AB  $[\text{Fe}_2(\text{BPMP})\{\text{O}_2\text{P}(\text{OPh})_2\}_2]\text{X}$  (I; X = Cl,  $\text{BF}_4$ ,  $\text{BPh}_4$ ; HBPMP = 2,6-bis[(bis(2-pyridylmethyl)amino)methyl]-4-methylphenol) and  $[\text{Fe}_2(\text{BPCP})\{\text{O}_2\text{CC}_2\text{H}_5\}_2]\text{BPh}_4$  (II; HBPCP = 2,6-bis[(bis(2-pyridylmethyl)amino)methyl]-4-chlorophenol) were prepared to provide insight into the integer-spin EPR signals found in the diferrous forms of diiron-oxo proteins. I (X = Cl) crystallizes as triclinic, space group P.hivin.1,  $a$  10.464(8),  $b$  15.226(7),  $c$  20.050(10) Å,  $\alpha$  85.60(4),  $\beta$  88.38(5),  $\gamma$  74.98(5)°,  $Z$  = 2,  $R$  = 0.049,  $R_w$  = 0.069. It has a ( $\mu$ -phenoxo)bis( $\mu$ - **phosphato**)diiron core. II, like  $[\text{Fe}_2(\text{BPMP})\{\text{O}_2\text{CC}_2\text{H}_5\}_2]\text{BPh}_4$  (III), exhibits a low field EPR signal near  $g$  = 17, similar to that found for deoxyhemerythrin azide. This resonance originates from a ground electronic state with integer spin, indicating that the metal centers are ferromagnetically coupled. I differ in 2 respects. They show EPR signals at  $g$  = 15, a resonance position that is incompatible with both strong and weak coupling models earlier proposed to explain the corresponding signals in III. The EPR signals of I arise from an excited state; the coupling interaction between the Fe centers is antiferromagnetic. The temperature dependence of the EPR signal indexes that the excited state is 12 cm<sup>-1</sup> above the EPR silent ground state. These observations are corroborated by magnetization data for polycryst. I (X =  $\text{BF}_4$ ). The switch in sign of the Fe-Fe coupling interaction on going from the propionate-bridged complexes to the **phosphate**-bridged complexes undoubtedly results from the larger Fe- $\mu$ -O-Fe angle found in

the latter complexes. The EPR properties observed for these complexes serve to validate the theor. framework proposed by H. et al. (ibid., 1991) to rationalize the integer-spin EPR signals observed for the diferrous forms of diiron-oxo proteins and provide a foundation upon which to interpret the  $g = 15$  signal recently observed for the diferrous R2 protein of ribonucleotide reductase.

- CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 7, 75, 77
- ST crystal structure iron **phosphato** pyridylmethylaminomethylmethylphenolato dinuclear; ESR iron pyridylmethylaminomethylphenolato **phosphato** propionato dinuclear
- IT **146436-30-8P**  
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(formation and reaction of, with ferrous **fluoroborate**)
- IT 9047-64-7, Ribonucleotide reductase  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(iron **diphenylphosphato** bis[(bis(pyridylmethyl)amino)methyl]methylphenolato dinuclear complex as model for diferrous R2 protein of)
- IT **146804-34-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ESR and magnetization of)
- IT **146600-73-9P 146804-35-5P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ESR of)
- IT **146804-33-3P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure and ESR of)
- IT **128328-49-4P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)
- IT **80528-41-2**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ferrous salts)
- IT **146436-30-8P**  
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(formation and reaction of, with ferrous **fluoroborate**)
- RN 146436-30-8 CAPLUS
- CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino)methyl]-4-chloro- (9CI) (CA INDEX NAME)



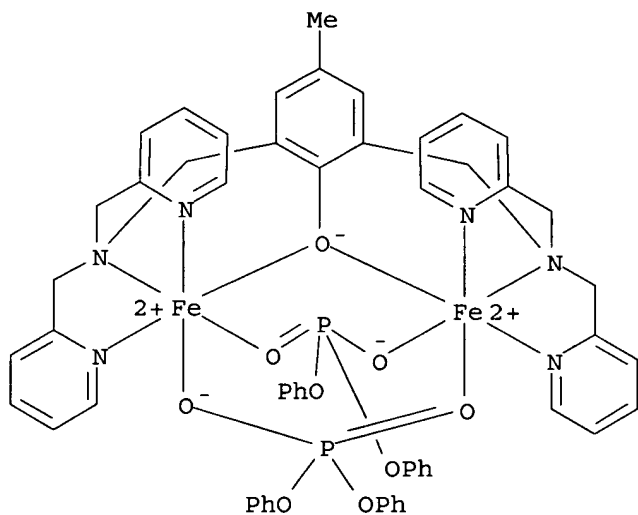
- IT **146804-34-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ESR and magnetization of)



RN 146804-34-4 CAPLUS  
 CN Iron(1+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(diphenyl phosphato-O':O'')]di-, stereoisomer, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

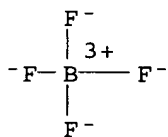
CM 1

CRN 126876-03-7  
 CMF C57 H53 Fe2 N6 O9 P2  
 CCI CCS



CM 2

CRN 14874-70-5  
 CMF B F4  
 CCI CCS

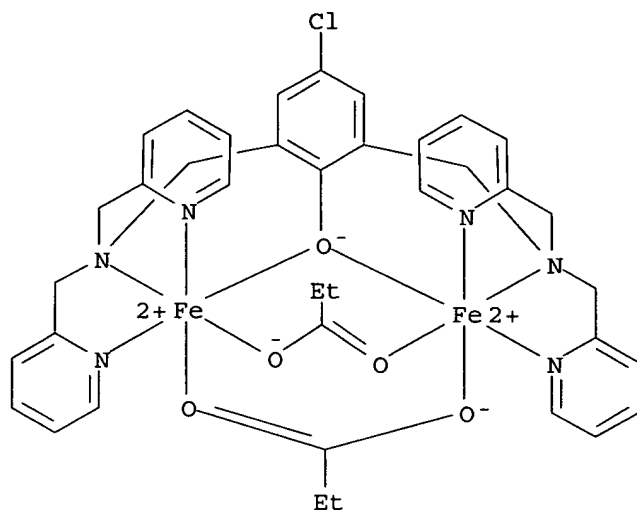


IT 146600-73-9P 146804-35-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and ESR of)  
 RN 146600-73-9 CAPLUS  
 CN Iron(1+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-chlorophenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(propanoato-O:O')]di-, stereoisomer, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 146600-72-8  
 CMF C38 H40 Cl Fe2 N6 O5

CCI CCS

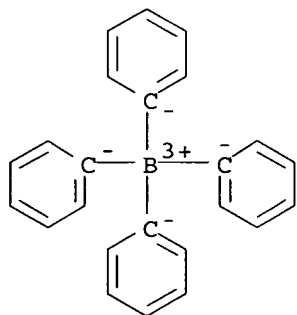


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



RN 146804-35-5 CAPLUS

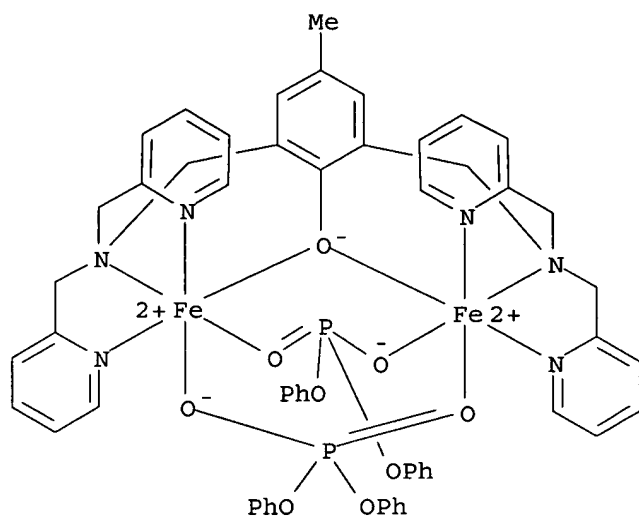
CN Iron(1+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(diphenylphosphato-O':O'')]di-, stereoisomer, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 126876-03-7

CMF C57 H53 Fe2 N6 O9 P2

CCI CCS

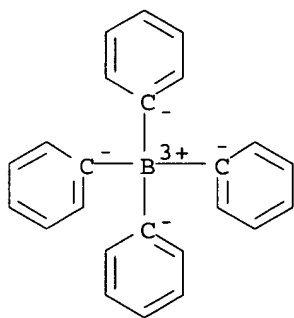


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



IT 146804-33-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure and ESR of)

RN 146804-33-3 CAPLUS

CN Iron(1+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(diphenylphosphato-O''':O''')]di-, stereoisomer, chloride, compd. with dichloromethane (1:2), monohydrate (9CI) (CA INDEX NAME)

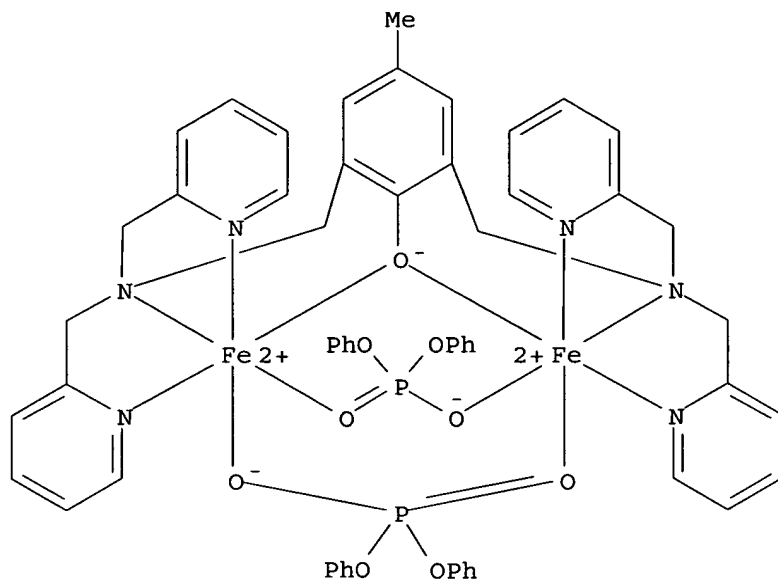
CM 1

CRN 146804-32-2

CMF C57 H53 Fe2 N6 O9 P2 . Cl

CCI CCS

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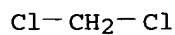
PAGE 2-A



CM 2

CRN 75-09-2

CMF C H2 Cl2



IT 128328-49-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 128328-49-4 CAPLUS

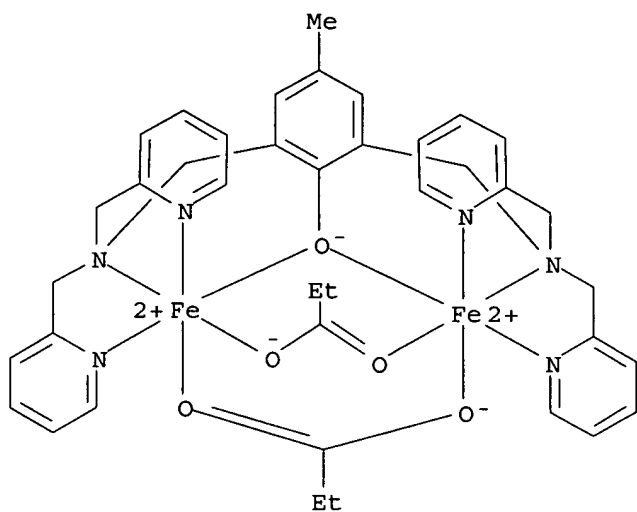
CN Iron(1+), [ $\mu$ -[2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methylphenolato-N2,N2',N2'',O1:N6,N6',N6'',O1]]bis[ $\mu$ -(propanoato-O:O')]di-, stereoisomer, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 121674-86-0

CMF C39 H43 Fe2 N6 O5

CCI CCS

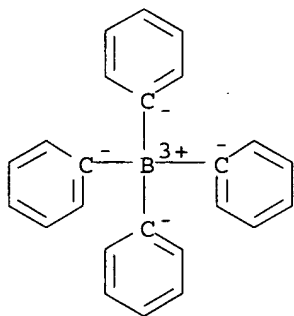


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS

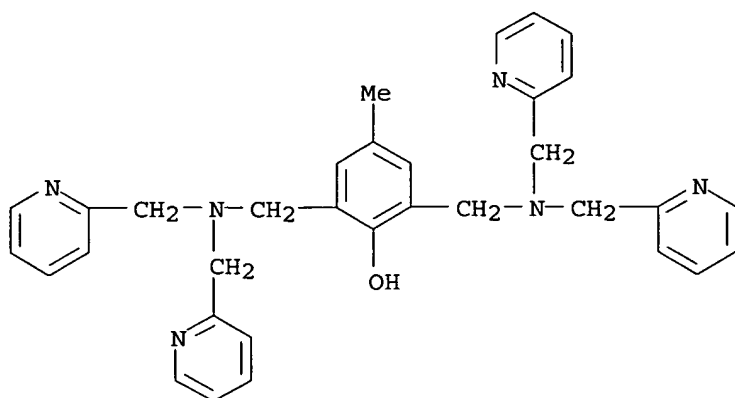


IT 80528-41-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ferrous salts)

RN 80528-41-2 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methyl- (9CI) (CA  
INDEX NAME)



L79 ANSWER 51 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:178768 CAPLUS

DOCUMENT NUMBER: 118:178768

TITLE: Formation of cryptatium species in solution:  
electrochemistry of bipyridyl-, bipyrimidyl-, and  
bithiazole-based cryptates

AUTHOR(S): Echegoyen, Luis; Perez-Cordero, Eduardo; Regnouf de  
Vains, Jean Bernard; Roth, Christine; Lehn, Jean Marie

CORPORATE SOURCE: Dep. Chem., Univ. Miami, Coral Gables, FL, 33124, USA

SOURCE: Inorganic Chemistry (1993), 32(5), 572-7

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB As a consequence of the recent success in isolating and characterizing the first crystalline cryptatium species, the redox properties of a series of cryptates have been analyzed in DMF using cyclic voltammetry. A total of eight cryptates, derived from six cryptands, were studied. These were the Na<sup>+</sup>, Ca<sup>2+</sup>, and La<sup>3+</sup> cryptates of tris(bipyridyl) (1-Na<sup>+</sup>, 1-Ca<sup>2+</sup>, 1-La<sup>3+</sup>) and the Na<sup>+</sup> complexes of the 5 other ligands, 2-6. Except for 6-Na<sup>+</sup> (bipyridyl-based), which exhibited irreversible behavior, and for 2-Na<sup>+</sup> (bithiazole-based), which, as expected, had only one redox couple, all of the cryptates showed at least three quasi-reversible redox couples. For 1-La<sup>3+</sup> a total of six cathodic waves were observed. A pronounced effect was observed for the reduction potentials when the central metal cation of the cryptate was changed. Thus for 1-Na<sup>+</sup> the first reduction potential occurs at -2.40 V (vs. ferrocene/ferrocenium, Fc/Fc<sup>+</sup>), while the corresponding value for 1-La<sup>3+</sup> is -1.76 V. On the other hand, for all of the Na<sup>+</sup> cryptates, the redox potential of each of the individual substituent groups (bipyridyl, bithiazole, dimethylbipyrimidine) was approx. independent of the other substituents present in the mol., although the reduction state of the complex affected these potentials. For example, the reduction potential for the bithiazole groups was the same for the sodium complexes of 2 and 3 (bipyridyl- and bithiazole-based) and almost the same for the first reduction of 4-Na<sup>+</sup> (bithiazole-based). Similarly, the reduction of the two bipyridyls of 3 and 5 (bipyridyl- and bipyrimidyl-based) occurred at the same potentials as those observed for the second and third redns. of 1-Na<sup>+</sup>. All of the reported redox processes correspond to ligand-centered orbitals, not to those of the metals, a result consistent with the spatially-isolated orbital theory which is accepted for bipyridyl complexes of Ru<sup>2+</sup>.

CC 72-2 (Electrochemistry)

Section cross-reference(s): 78

IT 3109-63-5, Tetrabutylammonium hexafluorophosphate

RL: PRP (Properties)  
(electrochem. reduction of sodium and calcium and lanthanum cryptates in DMF containing)

IT 7789-41-5, Calcium bromide (CaBr<sub>2</sub>) 134055-00-8

RL: PRP (Properties)  
(in preparation of calcium cryptate bromide)

IT 113597-85-6 113597-86-7 146841-19-2  
146864-88-2 146873-34-9 146873-35-0 146873-36-1  
146873-37-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of, electrochem., in DMF on glassy carbon)

IT 134055-00-8

RL: PRP (Properties)  
(in preparation of calcium cryptate bromide)

RN 134055-00-8 CAPLUS

CN Sodium(1+), (1,14,39,40,41,42,43,44-octaazaocryptacyclo[12.12.12.13,7.18,12.16,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-κN1,κN14,κN39,κN40,κN41,κN42,κN43,κN44)-, bromide, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)

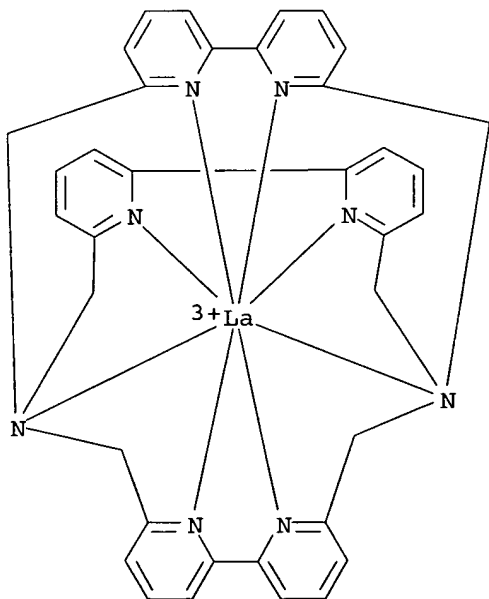
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 113597-85-6 113597-86-7 146864-88-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of, electrochem., in DMF on glassy carbon)

RN 113597-85-6 CAPLUS

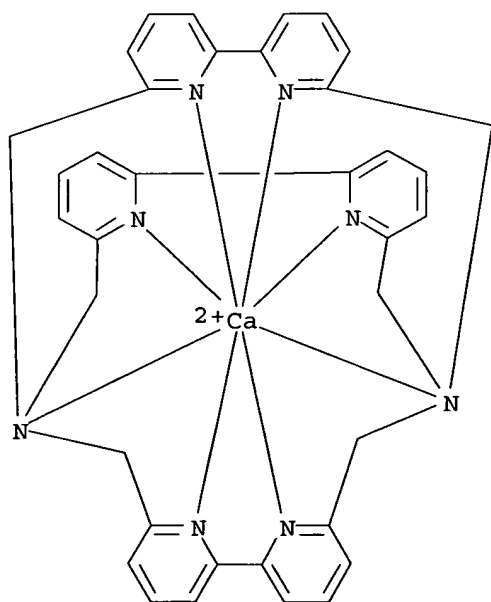
CN Lanthanum(3+), (1,14,39,40,41,42,43,44-octaazaocryptacyclo[12.12.12.13,7.18,12.16,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-N1,N14,N39,N40,N41,N42,N43,N44)-, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



RN 113597-86-7 CAPLUS

CN Sodium(1+), (1,14,39,40,41,42,43,44-octaazaocryptacyclo[12.12.12.13,7.18,12.16,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-

|    |  |        |
|----|--|--------|
| RN | 146864-88-2  | CAPLUS |
| CN | Calcium(2+), (1,14,39,40,41,42,43,44-octaazaoctacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-N1,N14,N39,N40,N41,N42,N43,N44)-, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME) |        |



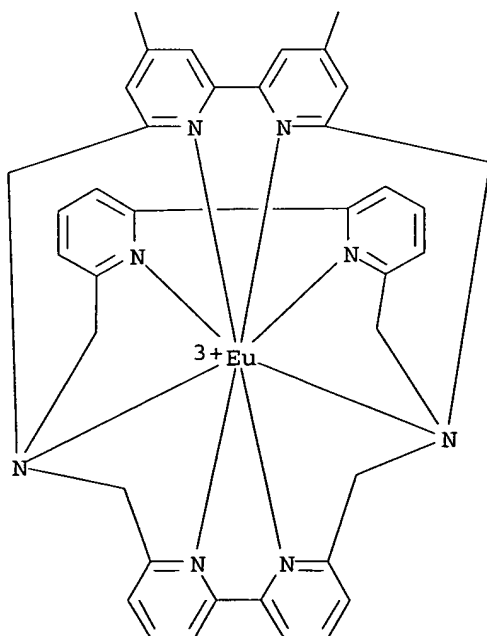


ACCESSION NUMBER: 1992:435802 CAPLUS  
DOCUMENT NUMBER: 117:35802  
TITLE: Luminescence of lanthanide cryptates: effects of  
**phosphate** and iodide anions  
AUTHOR(S): Sabbatini, Nanda; Guardigli, Massimo; Lehn, Jean  
Marie; Mathis, Gerard  
CORPORATE SOURCE: Dip. Chim. "G. Ciamician", Univ. Bologna, Bologna,  
40126, Italy  
SOURCE: Journal of Alloys and Compounds (1992), 180, 363-7  
CODEN: JALCEU; ISSN: 0925-8388  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The dependence of the luminescence of lanthanide cryptates on the  
interaction with the environment is examined. Anionic species can influence  
the luminescence by either entering the 1st coordination sphere of the  
metal ion or by giving rise to bimol. processes. These effects are  
investigated on systems containing Eu<sup>3+</sup> or Tb<sup>3+</sup> cryptates and I<sup>-</sup> or PO<sub>4</sub><sup>3-</sup>.  
The results are discussed on the basis of the nature of the lanthanide ion  
and the ligand-metal interaction in the excited state.  
CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related  
Properties)  
ST luminescence lanthanide cryptate effect iodide **phosphate**  
IT 14265-44-2, **Phosphate**, properties 20461-54-5, Iodide,  
properties  
RL: PRP (Properties)  
(luminescence of lanthanide cryptates in presence of)  
IT 65013-29-8 71238-22-7 107539-34-4 **125433-99-0**  
RL: PRP (Properties)  
(luminescence of, anion effects on)  
IT **125433-99-0**  
RL: PRP (Properties)  
(luminescence of, anion effects on)  
RN 125433-99-0 CAPLUS  
CN Europium(3+), (dimethyl 1,14,39,40,41,42,43,44-  
octaazaooctacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetr  
aconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,  
37(39)-octadecaene-5,10-dicarboxylate-κN1,κN14,κN39,.kap  
pa.N40,κN41,κN42,κN43,κN44) - (9CI) (CA INDEX  
NAME)

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$$\Rightarrow \Rightarrow$$

=> file registry

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STRUCTURE  
SEARCH  
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STRUCTURE FILE UPDATES: 26 MAR 2006 HIGHEST RN 878044-67-8

DICTIONARY FILE UPDATES: 26 MAR 2006 HIGHEST RN 878044-67-8

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Considered.  
04/28/06  
MEC

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

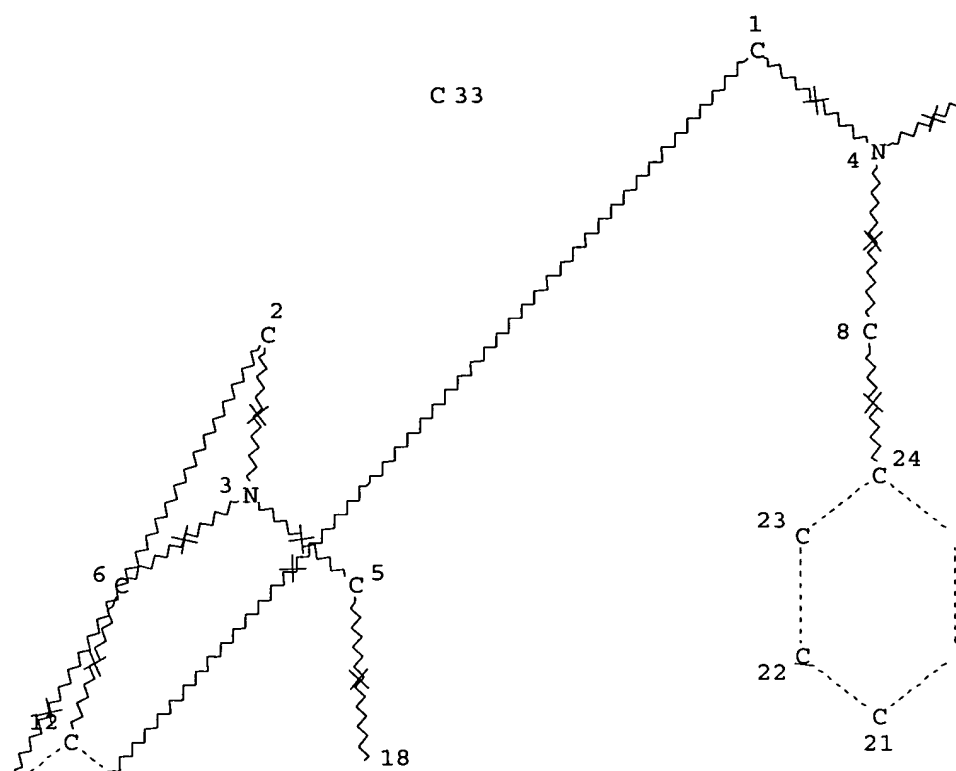
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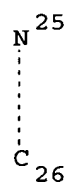
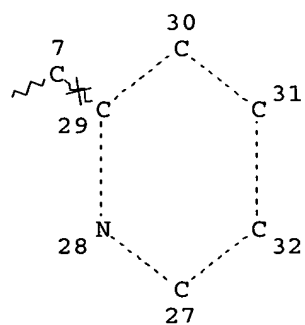
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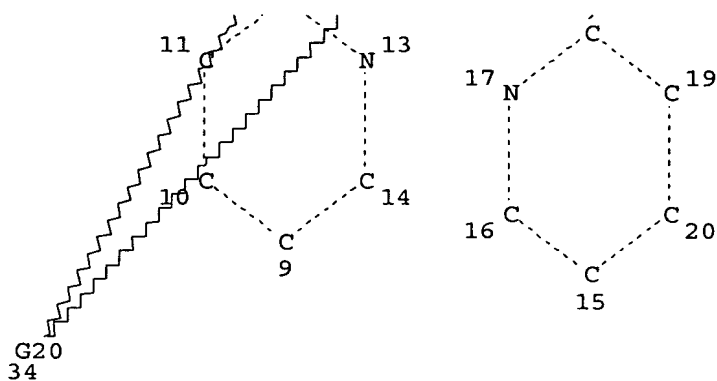
L7 STR



Page 1-A



Page 1-B



Page 2-A

REP G20=(2-10) 33-2 33-1

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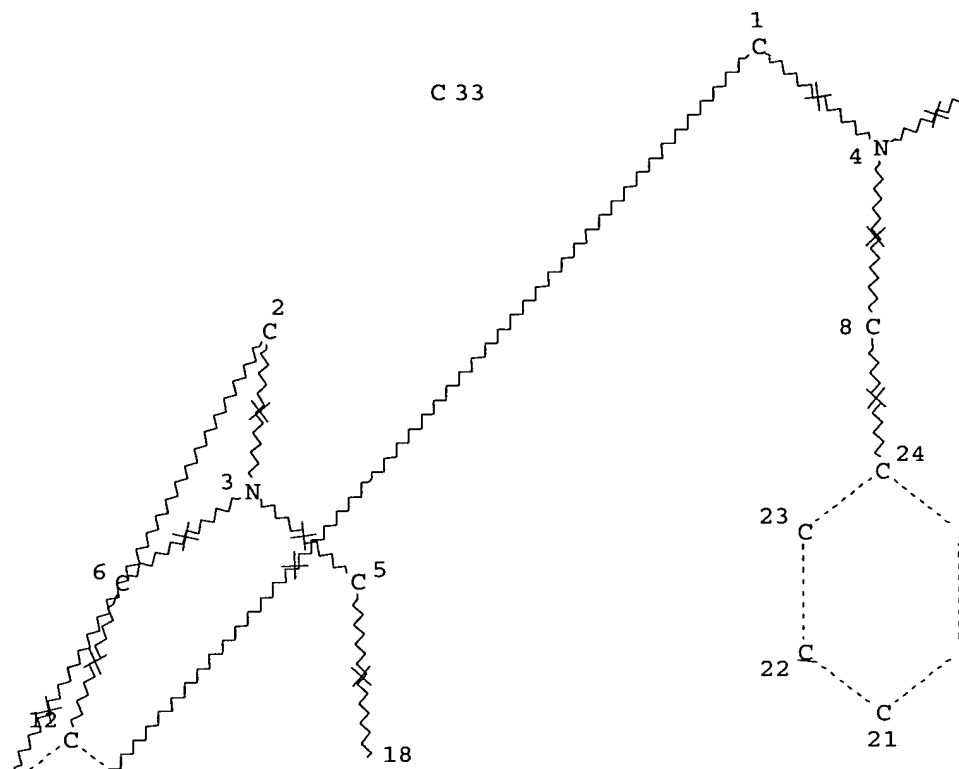
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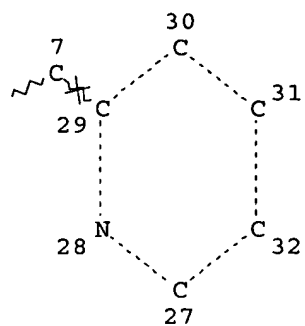
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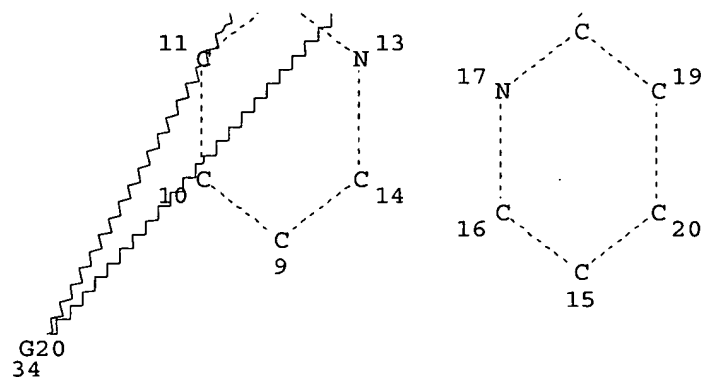
1261 ANSWERS

=> d stat que L19  
L7 STR

Page 1-A



Page 1-B



Page 2-A

REP G20=(2-10) 33-2 33-1

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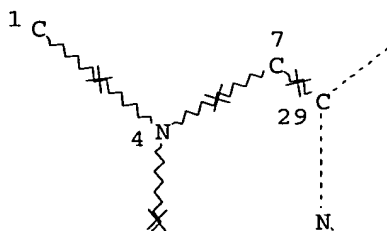
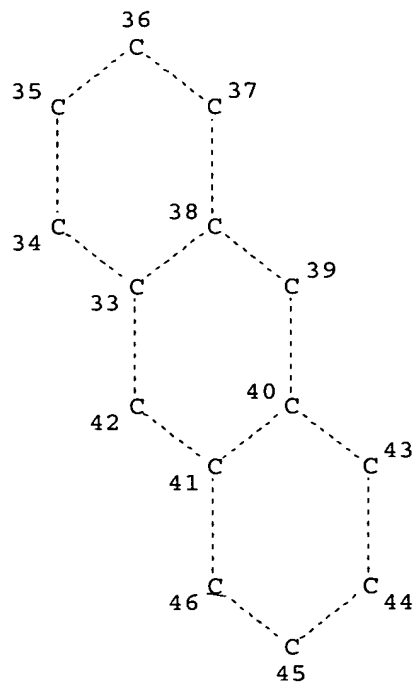
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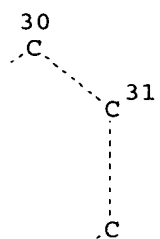
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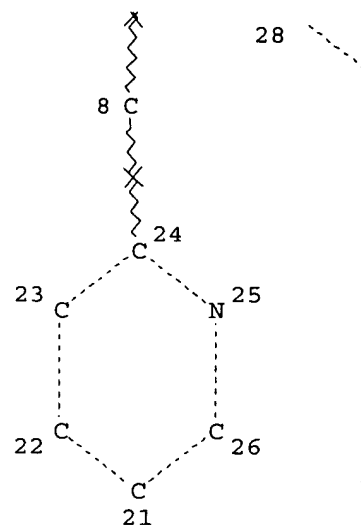
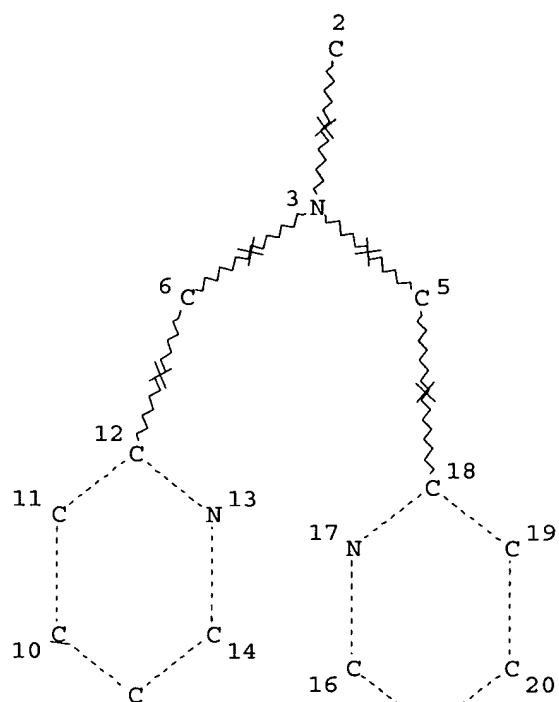




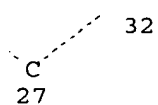
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Page 1-B



Page 2-A



Page 2-B



Page 3-A

NODE ATTRIBUTES:

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MLEVEL IS CLASS AT 1 2 3 4 5 6 7 8  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE  
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100.0% PROCESSED 72 ITERATIONS  
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14 ANSWERS

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FILE 'CAPLUS' ENTERED AT 13:28:12 ON 27 MAR 2006

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AUTHOR SEARCH

=> d que nos L58

|     |  |
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| L11 | 1261 SEA FILE=REGISTRY SSS FUL L7              |
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| L58 | 5 SEA FILE=CAPLUS ABB=ON PLU=ON L13 AND L57    |

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L58 ANSWER 1 OF 5 CAPLUS /COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:601921 CAPLUS

DOCUMENT NUMBER: 143:262802

TITLE: Indicator displacement assays that detect bilayer membranes enriched in phosphatidylserine

AUTHOR(S): Hanshaw, Roger G.; O'Neil, Edward J.; Foley, Meredith; Carpenter, Rachael T.; **Smith, Bradley D.**

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA

SOURCE: Journal of Materials Chemistry (2005), 15(27-28), 2707-2713

CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three indicator displacement assays are described for the detection of phosphatidylserine in a bilayer membrane. A series of Zn<sup>2+</sup>-dipicolylamine coordination compds. are used to bind selectively to the phosphatidylserine and act as a colorimetric chemosensing ensemble when combined with the UV-Vis indicator pyrocatechol violet. A similar displacement assay uses a coumarin methylsulfonate derivative as a fluorescent indicator, and a third assay involves quenching of calcein fluorescence by Cu<sup>2+</sup> and subsequent fluorescence restoration upon addition of phosphatidylserine. In the best case, vesicle membranes containing as little as 5% phosphatidylserine could be detected under physiol. relevant conditions using as little as 10  $\mu$ M sensing ensemble, and two of the

three systems allow vesicles containing 50% phosphatidylserine to be detected by the naked eye.

CC 9-5 (Biochemical Methods)

IT 115-41-3, Pyrocatechol violet 1461-15-0, Calcein 7440-50-8, Copper, biological studies 19524-63-1 **676257-32-2** 676257-34-4 **813420-19-8** **813420-23-4**

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(indicator displacement assays that detect bilayer membranes enriched in phosphatidylserine)

IT **676257-32-2** **813420-19-8** **813420-23-4**

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(indicator displacement assays that detect bilayer membranes enriched in phosphatidylserine)

RN 676257-32-2 CAPLUS

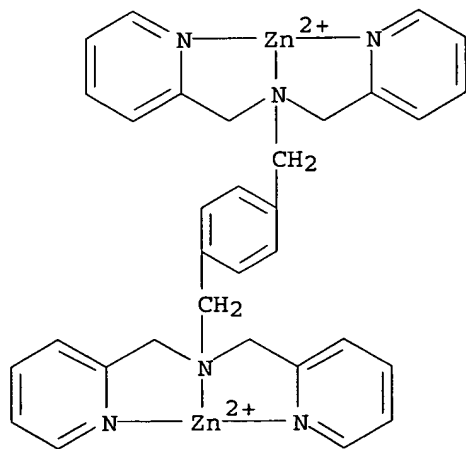
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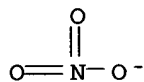
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CRN 14797-55-8

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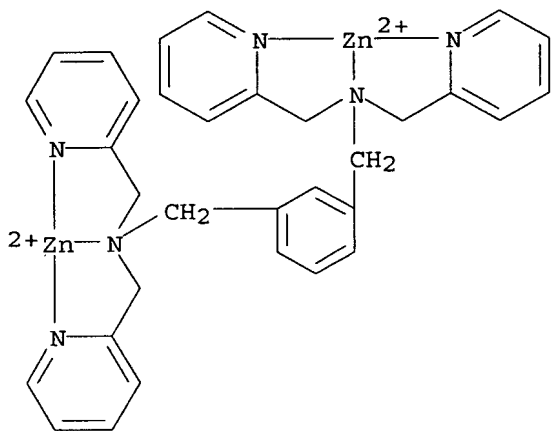
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INDEX NAME)

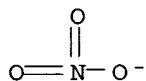
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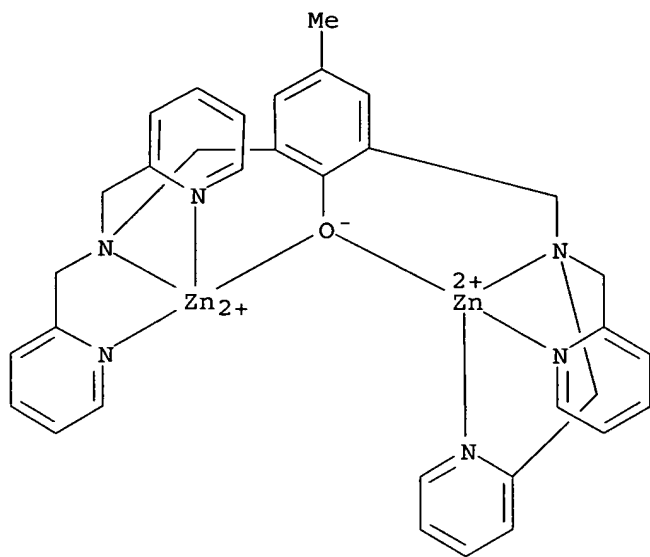
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RN 813420-23-4 CAPLUS  
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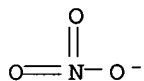
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 CCI CCS



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CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:430614 CAPLUS

DOCUMENT NUMBER: 143-188411

TITLE: Anion-Mediated Phase Transfer of Zinc(II)-Coordinated Tyrosine Derivatives

AUTHOR(S): Jiang, Hua; O'Neil, Edward J.; DiVittorio, Kristy M.; Smith, Bradley D.

CORPORATE SOURCE: Department of Chemistry Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA

SOURCE: Organic Letters (2005), 7(14), 3013-3016

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tyrosine-derived Zn<sup>2+</sup> coordination complexes and their fluorescent NBD conjugates are synthesized in a short, high-yielding procedure. The Zn<sup>2+</sup> complexes are highly water soluble, but in the presence of sodium laurate they readily transfer into an octanol layer. Furthermore, the NBD-labeled bis-Zn<sup>2+</sup> complex can partition into vesicle membranes containing anionic phospholipids.

CC 6-1 (General Biochemistry)

Section cross-reference(s): 34, 78

IT 861884-00-6P **861884-02-8P 861884-06-2P**  
 RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (zinc-coordinated dipicolylamine tyrosine derivs. preparation and sodium laurate-mediated transfer into octanol layers and NBD-labeled analog partitioning into membranes containing anionic phospholipids)

IT 861844-74-8P **861844-75-9P** 861844-76-0P **861844-77-1P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (zinc-coordinated dipicolylamine tyrosine derivs. preparation and sodium laurate-mediated transfer into octanol layers and NBD-labeled analog partitioning into membranes containing anionic phospholipids)

IT **861884-02-8P 861884-06-2P**  
 RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (zinc-coordinated dipicolylamine tyrosine derivs. preparation and sodium laurate-mediated transfer into octanol layers and NBD-labeled analog partitioning into membranes containing anionic phospholipids)

RN 861884-02-8 CAPLUS

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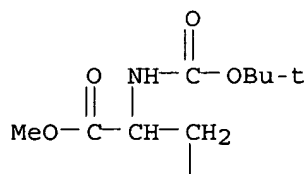
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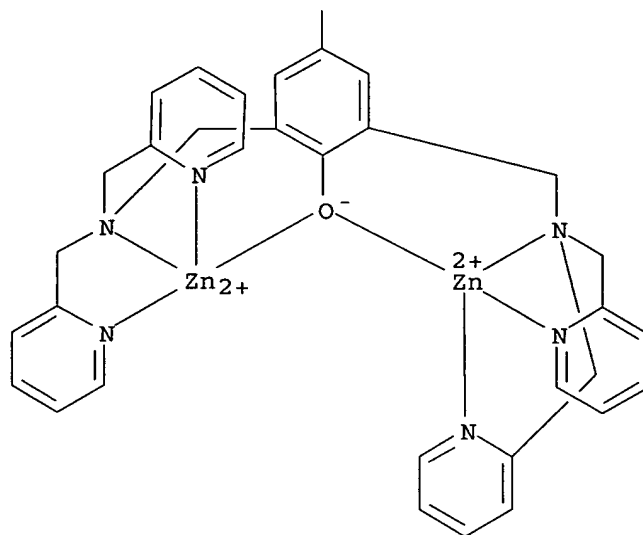
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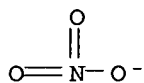
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CRN 14797-55-8

CMF N O3



RN 861884-06-2 CAPLUS

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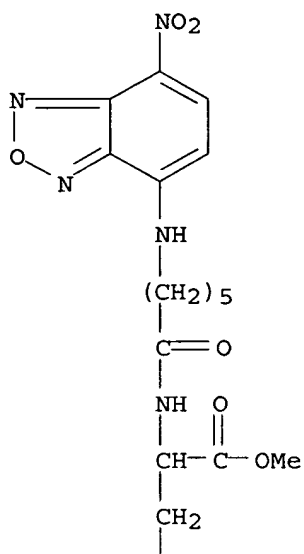
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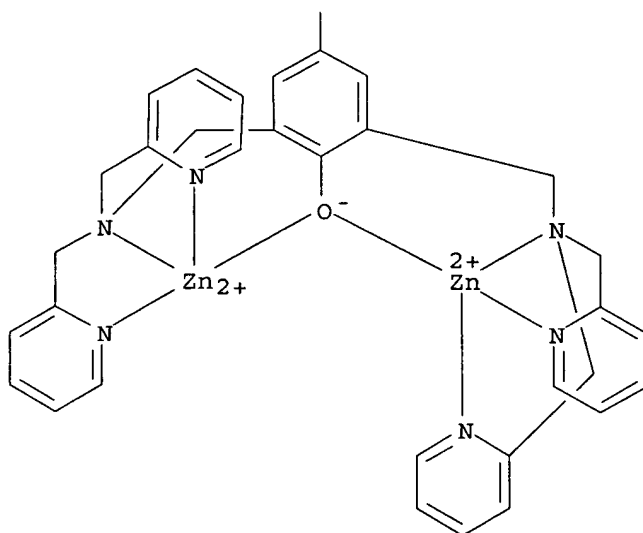
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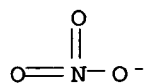
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CMF N O3



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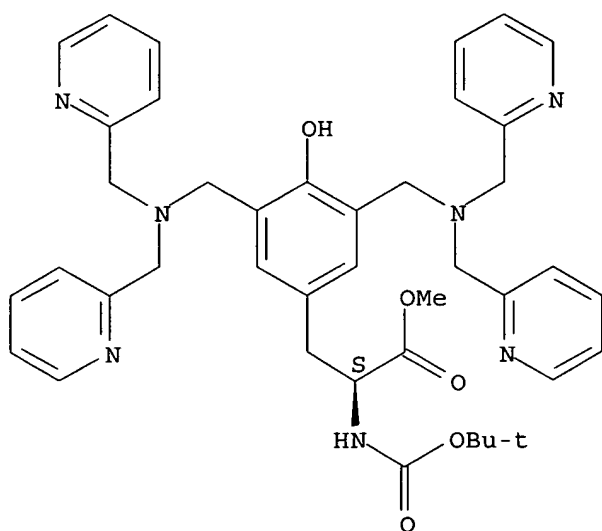
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(zinc-coordinated dipicolylamine tyrosine derivs. preparation and sodium laurate-mediated transfer into octanol layers and NBD-labeled analog partitioning into membranes containing anionic phospholipids)

RN 861844-75-9 CAPLUS

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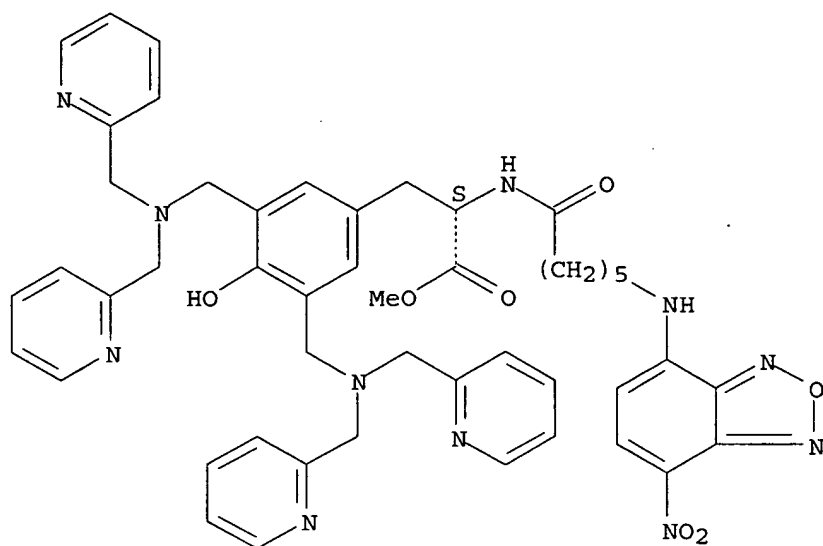
Absolute stereochemistry.



RN 861844-77-1 CAPLUS

CN L-Tyrosine, 3,5-bis[[bis(2-pyridinylmethyl)amino]methyl]-N-[6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-1-oxohexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:921771 CAPLUS

DOCUMENT NUMBER: 142:89070

TITLE: Fluorophore-linked zinc(II)dipicolylamine coordination complexes as sensors for phosphatidylserine-containing membranes

AUTHOR(S): Lakshmi, C.; Hanshaw, Roger G.; **Smith, Bradley D.**

CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Walther Center for Cancer Research, University of Notre Dame, Notre Dame, IN, 46556-5670, USA

SOURCE: Tetrahedron (2004), 60(49), 11307-11315

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:89070

AB A series of Zn<sup>2+</sup>-2,2'-dipicolylamine (Zn<sup>2+</sup>-DPA) coordination complexes with an attached NBD fluorophore are synthesized and evaluated as fluorescent sensors. The sensors do not respond to vesicles composed of zwitterionic phosphatidylcholine, but the NBD fluorescence emission is enhanced in the presence of anionic vesicles. A sensor with two Zn<sup>2+</sup>-DPA units and a hydrophilic tris(ethyleneoxy) linker produced a larger emission enhancement than an analog with a Bu linker, and titration with 1:1 POPC:POPS vesicles lead to an apparent phospholipid association constant of 5.3+104 M<sup>-1</sup>. The sensor can detect the presence of vesicles containing as little as 5% phosphatidylserine. The sensing effect apparently requires a membrane surface because the sensors do not respond to a phosphatidylserine derivative that is monodispersed in aqueous solution

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 6, 67

IT 819077-20-8P 819077-22-0P 819077-24-2P 819077-26-4P

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(fluorophore-linked zinc(II)dipicolylamine coordination complexes as

sensors for phosphatidylserine-containing membranes)

IT 819066-95-0P 819066-96-1P **819066-97-2P** 819066-98-3P  
**819066-99-4P** 819067-00-0P 819067-01-1P **819067-02-2P**  
**819067-03-3P** 819067-04-4P 819067-05-5P 819067-06-6P  
 819067-07-7P 819067-08-8P 819067-09-9P 819067-10-2P 819067-11-3P  
**852486-81-8P** 852486-86-3P 852533-78-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorophore-linked zinc(II)dipicolylamine coordination complexes as sensors for phosphatidylserine-containing membranes)

IT **819077-20-8P** **819077-22-0P**

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(fluorophore-linked zinc(II)dipicolylamine coordination complexes as sensors for phosphatidylserine-containing membranes)

RN 819077-20-8 CAPLUS

CN Zinc(4+), [ $\mu$ -[5-[4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]butoxy]-N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-1,3-benzenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

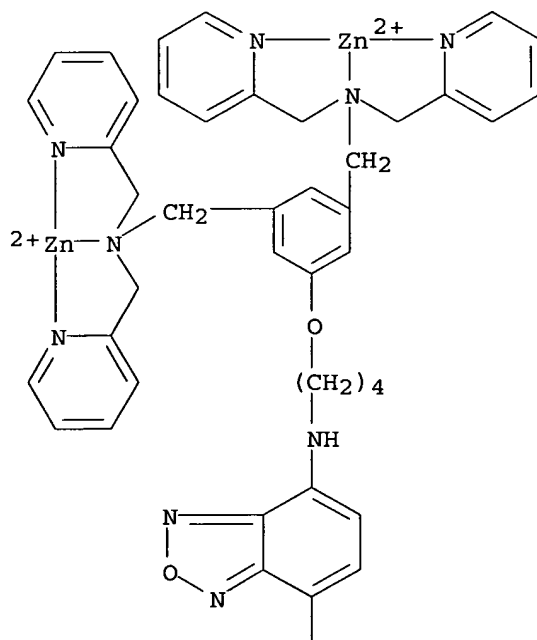
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CRN 819077-19-5

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CCI CCS

PAGE 1-A



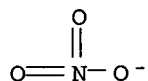
PAGE 2-A



CM 2

CRN 14797-55-8

CMF N O3



RN 819077-22-0 CAPLUS

CN Zinc(4+), [ $\mu$ -[5-[2-[2-[2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethoxy]ethoxy]ethoxy]-N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-1,3-benzenedimethanamine- $\kappa$ N: $\kappa$ N']]]di-, tetranitrate (9CI) (CA INDEX NAME)

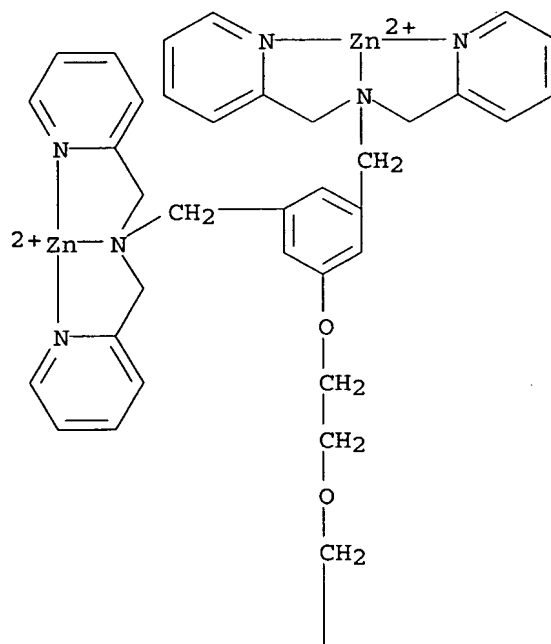
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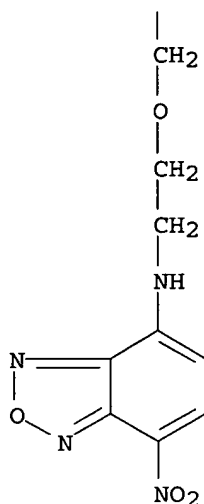
CMF C44 H46 N10 O6 Zn2

CCI CCS

PAGE 1-A



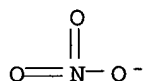
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CM 2

CRN 14797-55-8

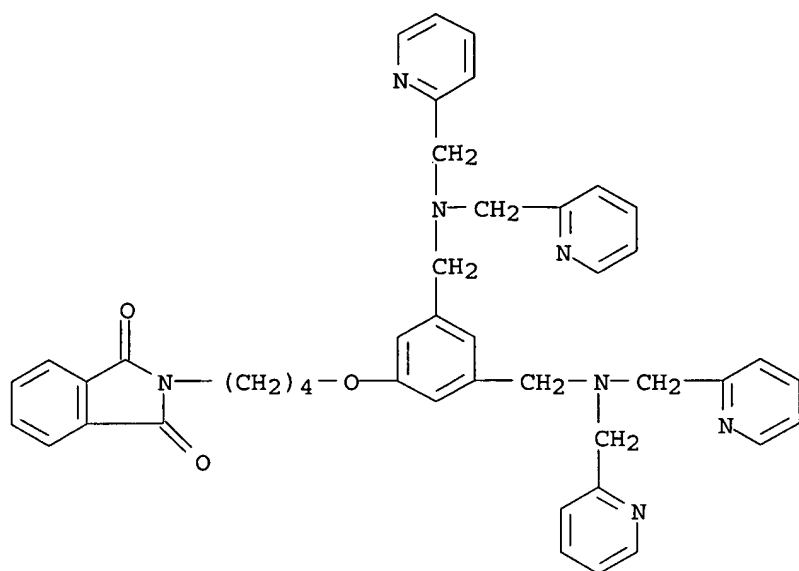
CMF N O3



IT 819066-97-2P 819066-98-3P 819066-99-4P  
 819067-02-2P 819067-03-3P 852486-81-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (fluorophore-linked zinc(II)dipicolylamine coordination complexes as  
 sensors for phosphatidylserine-containing membranes)

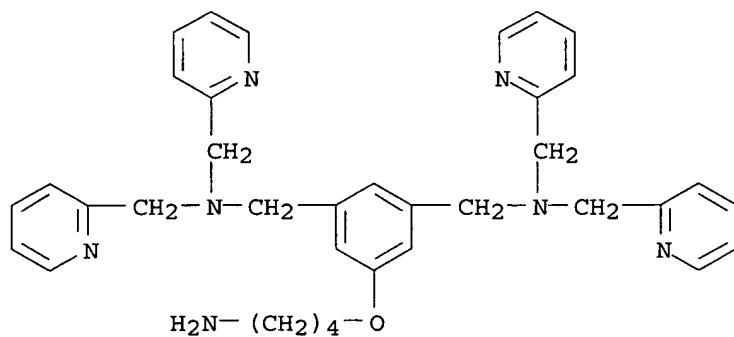
RN 819066-97-2 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[3,5-bis[[bis(2-  
 pyridinylmethyl)amino]methyl]phenoxy]butyl]- (9CI) (CA INDEX NAME)



RN 819066-98-3 CAPLUS

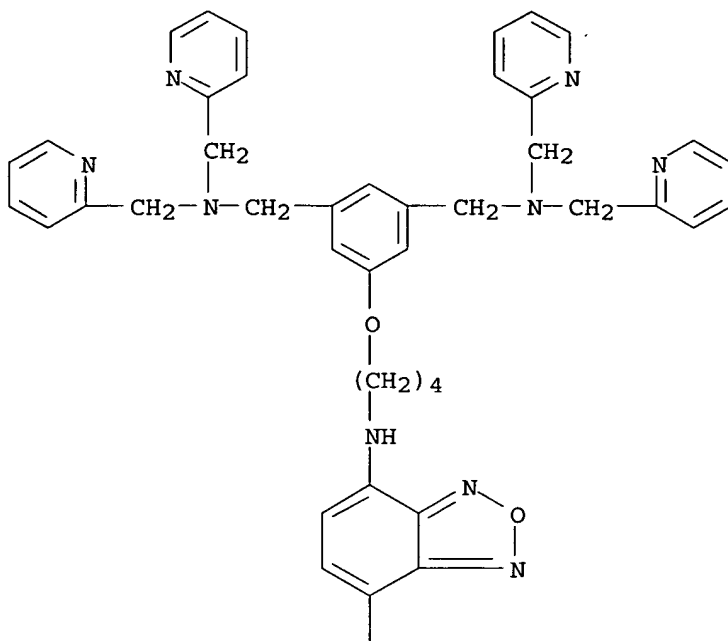
CN 1,3-Benzenedimethanamine, 5-(4-aminobutoxy)-N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 819066-99-4 CAPLUS

CN 1,3-Benzenedimethanamine, 5-[4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]butoxy]-N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

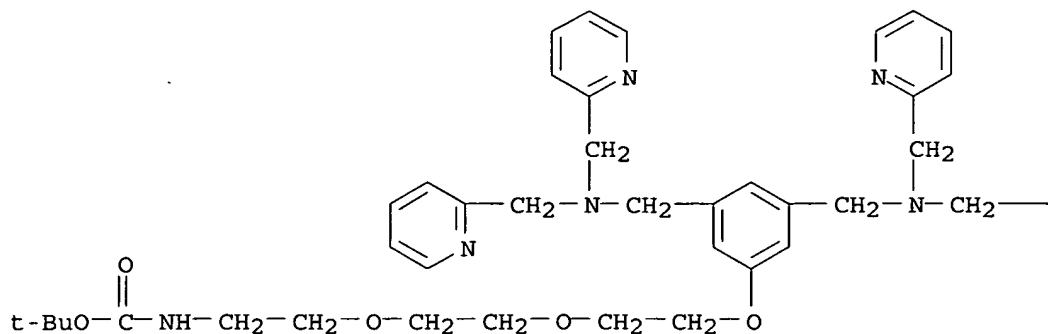


PAGE 2-A



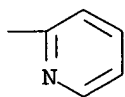
RN 819067-02-2 CAPLUS  
 CN Carbamic acid, [2-[2-[2-[3,5-bis[[bis(2-pyridinylmethyl)amino]methyl]phenoxy]ethoxy]ethoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



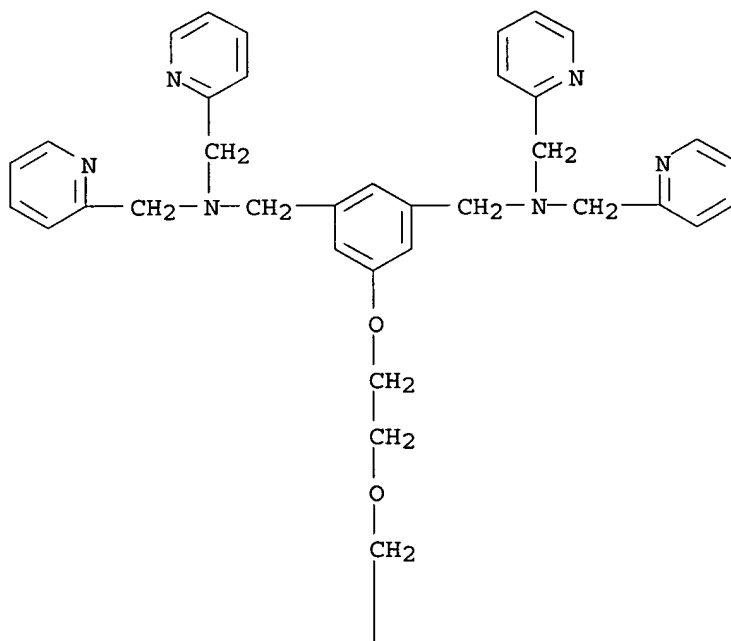


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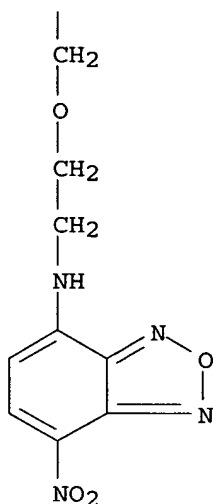


RN 819067-03-3 CAPLUS  
CN 1,3-Benzenedimethanamine, 5-[2-[2-[2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethoxy]ethoxy]ethoxy]-N,N,N',N'-tetrakis(2-pyridinylmethyl)-(9CI) (CA INDEX NAME)

PAGE 1-A

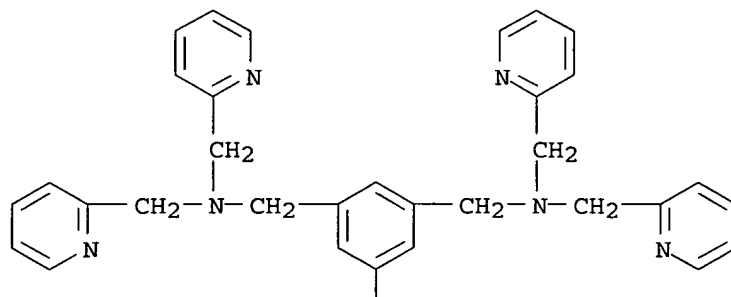


PAGE 2-A



RN 852486-81-8 CAPLUS

CN 1,3-Benzenedimethanamine, 5-[2-[2-(2-aminoethoxy)ethoxy]ethoxy]-N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

H<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-O-CH<sub>2</sub>-CH<sub>2</sub>-O-CH<sub>2</sub>-CH<sub>2</sub>-O

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:880433 CAPLUS

DOCUMENT NUMBER: 142:70992

TITLE: An indicator displacement system for fluorescent detection of phosphate oxyanions under physiological conditions

AUTHOR(S): Hanshaw, Roger G.; Hilkert, Sarah M.; Jiang, Hua; Smith, Bradley D.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA

SOURCE: Tetrahedron Letters (2004), 45(47), 8721-8724  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:70992

AB A fluorogenic chemosensing system is described and shown to selectively detect pyrophosphate under physiol. conditions. In the best case, pyrophosphate and hydrogen phosphate are capable of displacing a fluorescent coumarin-derived indicator from a bis Zn<sup>2+</sup>-dipicolylamine coordination compound with association consts. of 107 and 105 M<sup>-1</sup>, resp.

CC 9-5 (Biochemical Methods)

IT 305-01-1 14066-19-4, Hydrogen phosphate, uses 19524-62-0  
 676257-32-2 676257-34-4 813420-19-8  
 813420-23-4  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (indicator displacement system for fluorescent detection of phosphate oxyanions under physiol. conditions)

IT 676257-32-2 813420-19-8 813420-23-4  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (indicator displacement system for fluorescent detection of phosphate oxyanions under physiol. conditions)

RN 676257-32-2 CAPLUS

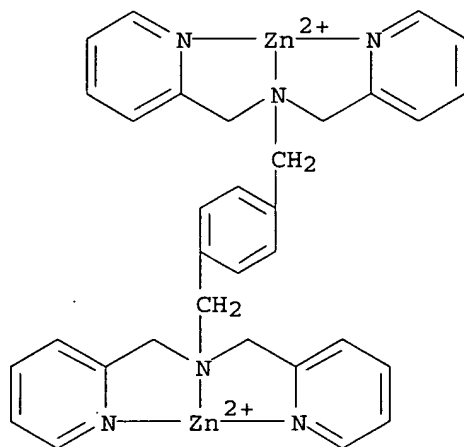
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-1,4-benzenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

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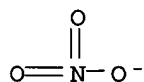
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



RN 813420-19-8 CAPLUS

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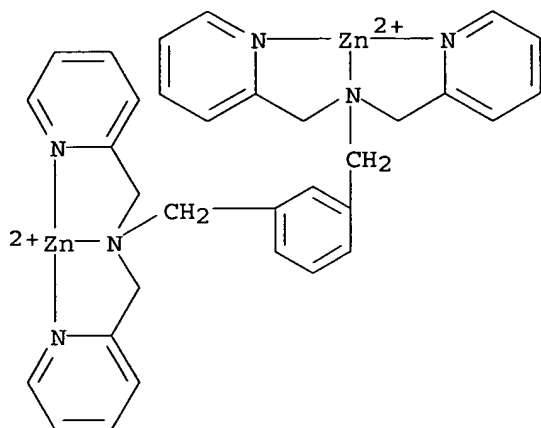
benzenedimethanamine- $\kappa N:\kappa N'$ ]]di-, tetranitrate (9CI) (CA INDEX NAME)

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CRN 813420-18-7

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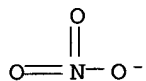
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CM 2

CRN 14797-55-8

CMF N O3



RN 813420-23-4 CAPLUS

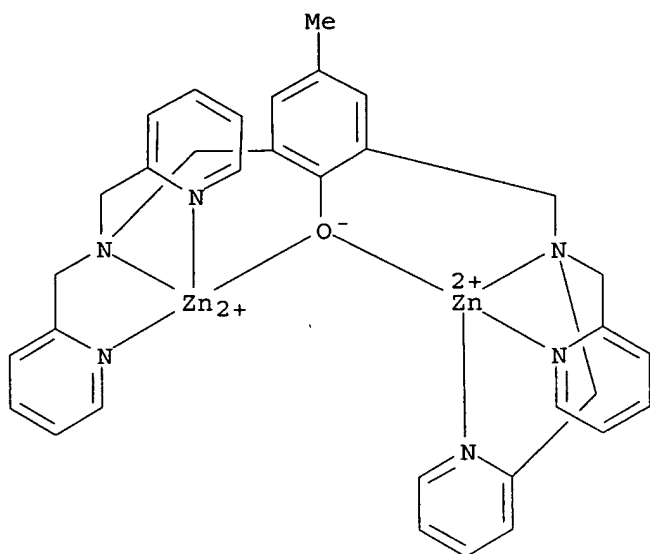
CN Zinc(3+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa N$ )methyl]amino- $\kappa N$ ]methyl]-4-methylphenolato- $\kappa O:\kappa O$ ]]di-, trinitrate (9CI) (CA INDEX NAME)

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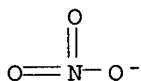
CRN 813420-22-3

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CCI CCS



CM 2

CRN 14797-55-8  
CMF N O3

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:904778 CAPLUS

DOCUMENT NUMBER: 141:170100

TITLE: Detection of apoptotic cells using a synthetic fluorescent sensor for membrane surfaces that contain phosphatidylserine

AUTHOR(S): Koulov, A. V.; Stucker, K. A.; Lakshmi, C.; Robinson, J. P.; Smith, B. D.

CORPORATE SOURCE: Walther Center for Cancer Research, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA

SOURCE: Cell Death and Differentiation (2003), 10(12), 1357-1359

CODEN: CDDIEK; ISSN: 1350-9047

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The membrane-binding and fluorescence-sensing properties of PSS-380, an anthracene derivative with two zinc dipicolylamine groups, were studied. PSS-380 was recently shown to bind phosphorylated compds. like phosphotyrosine in water with association consts. around 107 M<sup>-1</sup>. PSS-380 can sense the presence of anionic phospholipids, particularly

phosphatidylserine, on the surface of vesicles and cells. Furthermore, PSS-380 has the ability to act as a fluorescent sensor of apoptotic cells. A potential tech. drawback of PSS-380 is that it requires UV excitation, a feature that is presently not available to general flow cytometers.

CC 9-1 (Biochemical Methods)

Section cross-reference(s): 6

IT 439681-63-7, PSS 380

RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(PSS 380; detection of apoptotic cells using a synthetic fluorescent sensor for membrane surfaces that contain phosphatidylserine)

IT 439681-63-7, PSS 380

RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(PSS 380; detection of apoptotic cells using a synthetic fluorescent sensor for membrane surfaces that contain phosphatidylserine)

RN 439681-63-7 CAPLUS

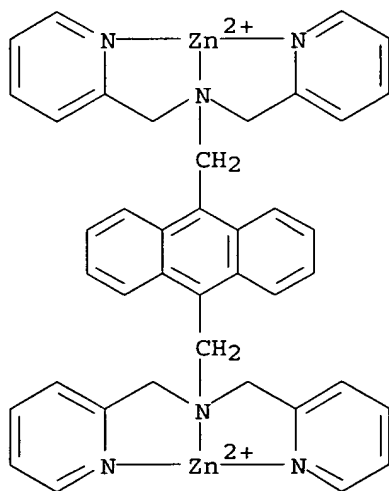
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

CM 1

CRN 360579-06-2

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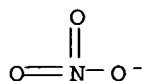
CCI  $\mu$ -ECS



CM 2

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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predicted properties as well as tags indicating availability of  
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*printed with author search*

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L77 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:673580 CAPLUS

DOCUMENT NUMBER: 143:301538

TITLE: Cooperation between Artificial Receptors and  
Supramolecular Hydrogels for Sensing and  
Discriminating **Phosphate** Derivatives



AUTHOR(S): Yamaguchi, Satoshi; Yoshimura, Ibuki; Kohira, Takahiro; Tamaru, Shunichi; Hamachi, Itaru  
CORPORATE SOURCE: PRESTO (Synthesis and Control Japan Science and Technology) Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Kyoto, 615-8510, Japan  
SOURCE: Journal of the American Chemical Society (2005), 127(33), 11835-11841  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB This study has successfully demonstrated that the cooperative action of artificial receptors with semi-wet supramol. hydrogels may produce a unique and efficient mol. recognition device not only for the simple sensing of **phosphate** derivs., but also for discriminating among **phosphate** derivs. The authors directly observed by confocal laser scanning microscopy that **fluorescent** artificial receptors can dynamically change the location between the aqueous cavity and the hydrophobic fibers upon guest-binding under semi-wet conditions provided by the supramol. hydrogel. On the basis of such a guest-dependent dynamic redistribution of the receptor mols., a sophisticated means for mol. recognition of **phosphate** derivs. can be rationally designed in the hydrogel matrix. That is, the elaborate utilization of the hydrophobic fibrous domains, as well as the water-rich hydrophilic cavities, enables the authors to establish three distinct signal transduction modes for **phosphate** sensing: the use of (i) a photoinduced electron transfer type of chemosensor, (ii) an environmentally sensitive probe, and (iii) an artificial receptor displaying a **fluorescence** resonance energy transfer type of **fluorescent** signal change. Thus, one can selectively sense and discriminate the various **phosphate** derivs., such as **phosphate**, **phospho**-tyrosine, **Ph phosphate**, and ATP, using a **fluorescence** wavelength shift and a seesaw type of ratiometric **fluorescence** change, as well as a simple **fluorescence** intensity change. It is also shown that an array of the miniaturized hydrogel is promising for the rapid and high-throughput sensing of these **phosphate** derivs.

CC 9-1 (Biochemical Methods)  
Section cross-reference(s): 28, 78

ST cooperation artificial receptor supramol hydrogel sensor **phosphate** deriv

IT Biosensors  
Confocal laser scanning microscopy  
Cooperative phenomena  
    **Fluorescence**  
    **Fluorescence** resonance energy transfer  
    **Fluorescent** indicators  
    **Fluorometry**  
High throughput screening  
Hydrogels  
Molecular association  
Molecular recognition  
Supramolecular structure  
    (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)

IT **Phosphates**, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
    (cooperation between artificial receptors and supramol. hydrogels for

- sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT Receptors  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV (Device component use); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT Optical sensors  
 (**fluorescent**; cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT Electron transfer  
 (photochem.; cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 439681-63-7  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV (Device component use); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (3cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 56-65-5, 5' ATP, analysis 60-92-4, CAMP 701-64-4, Phenyl **phosphate** 813-78-5, Dimethyl **phosphate** 14265-44-2, **Phosphate**, analysis 21820-51-9, **Phospho**-tyrosine  
 RL: ANT (Analyte); ANST (Analytical study)  
 (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 864738-95-4P 864738-97-6P  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV (Device component use); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 74-89-5, Methylamine, reactions 605-65-2, Dansyl chloride 1539-42-0, 2,2'-Dipicolylamine 7779-88-6, Zinc(II) nitrate 80883-54-1 200809-09-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 864685-58-5P 864685-59-6P 864685-60-9P 864685-61-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 473536-36-6  
 RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); DEV (Device component use); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (gelator; cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating **phosphate** derivs. in relation to synthesis of receptors)
- IT 439681-63-7  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); DEV

(Device component use); ANST (Analytical study); BIOL (Biological study);  
USES (Uses)

(3cooperation between artificial receptors and supramol. hydrogels for  
sensing and discriminating **phosphate** derivs. in relation to  
synthesis of receptors)

RN 439681-63-7 CAPLUS

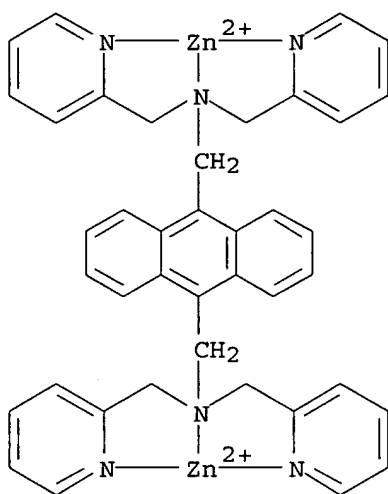
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-  
anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA  
INDEX NAME)

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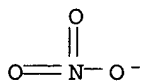
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

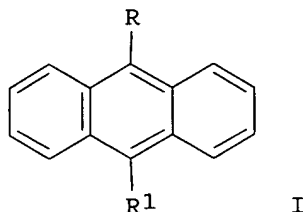
L77 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005 601954 CAPLUS

DOCUMENT NUMBER: 143:255917

TITLE: PET fluoroionophores for Zn2+ and Cu2+:  
complexation and fluorescence behavior of  
anthracene derivatives having diethylamine,  
N-methylpiperazine and N,N-bis(2-picoly)amine units  
AUTHOR(S): Kubo, Kanji; Mori, Akira

CORPORATE SOURCE: School of Dentistry, Health Sciences University of  
Hokkaido, Ishikari-Tobetsu, Japan  
SOURCE: Journal of Materials Chemistry (2005), 15(27-28),  
2902-2907  
CODEN: JMACEP; ISSN: 0959-9428  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

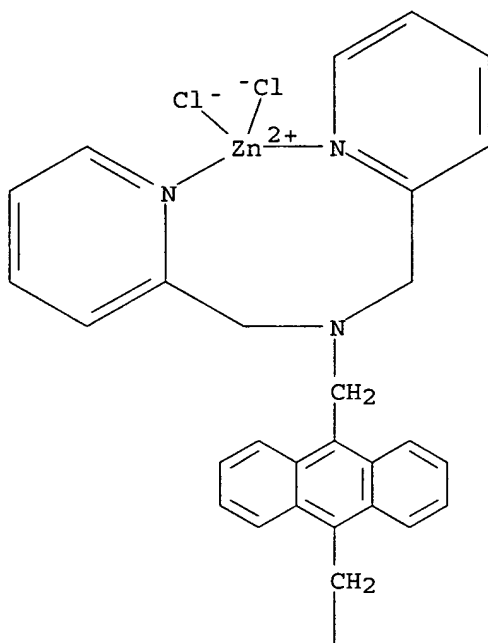


- AB Anthracene derivs. (I; R = CH<sub>2</sub>NEt<sub>2</sub>, N-methylpiperazinylmethyl, N,N-bis(2-dipicolyl)aminomethyl, R<sub>1</sub> = H (1); R = R<sub>1</sub> (2)) showed weak emission, suggesting that photoinduced electron transfer (PET) from the amine group to the excited anthracene occurs. The PET **fluoroionophores** (1, 2) display unique photophys. properties in the presence of the guest metal salts. Complexation of I (R = Et<sub>2</sub>N, N-methylpiperazinyl, R<sub>1</sub> = H; R = R<sub>1</sub> = Et<sub>2</sub>NCH<sub>2</sub>, N-methylpiperazinylmethyl) with Ni<sup>2+</sup>, Cu<sup>2+</sup> and Zn<sup>2+</sup> enhanced the emission, while the emission intensities of I (R = N,N-bis(2-picolyl)amino, R<sub>1</sub> = H; R = R<sub>1</sub> = N,N-bis(2-picolyl)aminomethyl) are increased in the presence of Zn<sup>2+</sup> and decreased in the presence of Ni<sup>2+</sup> and Cu<sup>2+</sup>. The crystal structures of I (R = R<sub>1</sub> = N,N-bis(2-picolyl)aminomethyl) and its Zn chloride complex showed that the binding of Zn<sup>2+</sup> to the N,N-bis(2-picolyl)aminomethyl unit inhibits the photoinduced electron transfer process. Intramol.  $\pi$ - $\pi$  interactions between anthracene and the ZnCl<sub>2</sub>-complexed pyridine were observed
- CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 68, 75
- ST zinc anthracene deriv complex prepn structure; crystal structure anthracene deriv zinc complex; assocn const anthracene deriv transition metal alk earth; **fluorescence** anthracene deriv transition metal effect
- IT **Fluorescence**  
(of anthracene diethylamino/methylpiperazinyl/bis(dipicolyl)amino derivs. with/without transition metals)
- IT 628297-15-4 863426-91-9  
RL: PRP (Properties)  
(crystal structure of)
- IT 35693-48-2 101296-96-2 190183-94-9 415923-37-4  
RL: PRP (Properties)  
(**fluorescence** and association consts. with transition metals)
- IT 108365-97-5 628297-13-2  
RL: PRP (Properties)  
(**fluorescence** and association consts. with transition metals and alkaline earth metals and crystal structure of)
- IT 628297-15-4  
RL: PRP (Properties)

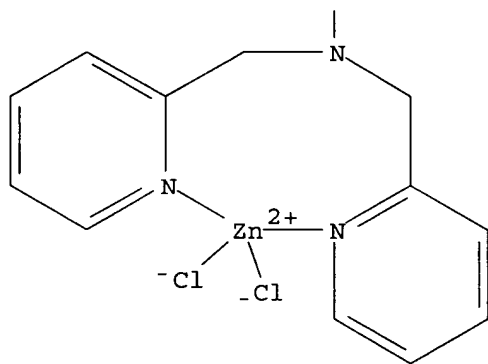
(crystal structure of)

RN 628297-15-4 CAPLUS  
 CN Zinc, tetrachloro[ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenediamine]]di- (9Cl) (CA INDEX NAME)

PAGE 1-A

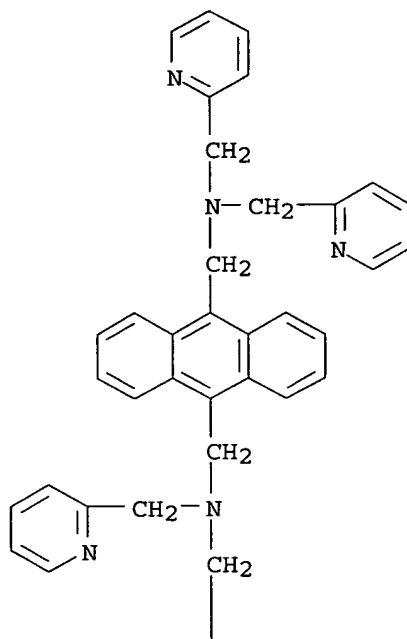


PAGE 2-A

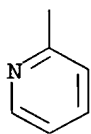


IT 628297-13-2  
 RL: PRP (Properties)  
 (fluorescence and association consts. with transition metals and alkaline earth metals and crystal structure of)  
 RN 628297-13-2 CAPLUS  
 CN 9,10-Anthracenedimethanamine, N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9Cl)  
 (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN  
 2004:729329 CAPLUS  
 141:419900  
 TITLE: Molecular recognition in a supramolecular hydrogel to afford a semi-wet sensor chip  
 AUTHOR(S): Yoshimura, Ibuki; Miyahara, Yoshifumi; Kasagi, Noriyuki; Yamane, Hiroki; Ojida, Akio; Hamachi, Itaru  
 CORPORATE SOURCE: PRESTO (Synthesis and Control JST) Institute for Materials Chemistry and Engineering (IMCE) and Department of Chemistry and Biochemistry, Kyushu University, Fukuoka, 812-8581, Japan  
 SOURCE: Journal of the American Chemical Society (2004), 126(39), 12204-12205  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB This communication describes a new mol. recognition chip using a semi-wet

microenvironment provided by a self-assembled hydrogel. From the evidence that the mol. recognition capability of artificial chemosensors are practically retained even in the hydrogel compared to those in aqueous solution,

the authors miniaturized the functionalized hydrogel to produce an unprecedented mol. recognition chip. Probably the present noncovalent immobilization method is generally applicable to many chemosensors, which leads to a unique semi-wet sensor chip suitable to convenient and high-throughput assay to plural analytes.

CC 80-2 (Organic Analytical Chemistry)

Section cross-reference(s): 79

IT **Fluorescence**

Molecular recognition

Optical sensors

pH

(mol. recognition in a supramol. hydrogel to afford a semi-wet sensor chip)

IT 701-64-4, Phenyl **phosphate** 12408-02-5, Hydrogen ion, analysis

14265-44-2, **Phosphate**, analysis 21820-51-9, **Phospho**-tyrosine

RL: ANT (Analyte); ANST (Analytical study)

(analyte; mol. recognition in a supramol. hydrogel to afford a semi-wet sensor chip)

IT 7439-95-4, Magnesium, analysis 7440-02-0, Nickel, analysis 7440-48-4, Cobalt, analysis 7440-50-8, Copper, analysis 7440-70-2, Calcium, analysis

RL: ARU (Analytical role, unclassified); PRP (Properties); ANST (Analytical study)

(divalent, analyte; effect on **fluorescence** of anthracene derivative receptor in presence of supramol. hydrogel)

IT 7440-09-7, Potassium, analysis 7440-23-5, Sodium, analysis

RL: ARU (Analytical role, unclassified); PRP (Properties); ANST (Analytical study)

(monovalent, analyte; effect on **fluorescence** of anthracene derivative receptor in presence of supramol. hydrogel)

IT **439681-63-7** 780763-75-9

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (receptor; mol. recognition in a supramol. hydrogel to afford a semi-wet sensor chip)

IT 7439-89-6, Iron, analysis

RL: ARU (Analytical role, unclassified); PRP (Properties); ANST (Analytical study)

(trivalent, analyte; effect on **fluorescence** of anthracene derivative receptor in presence of supramol. hydrogel)

IT **439681-63-7**

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (receptor; mol. recognition in a supramol. hydrogel to afford a semi-wet sensor chip)

RN 439681-63-7 CAPLUS

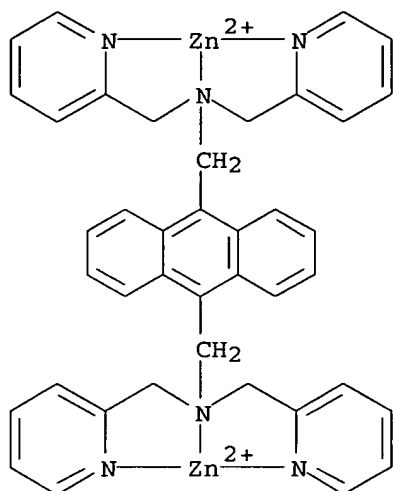
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

CM 1

CRN 360579-06-2

CMF C40 H36 N6 Zn2

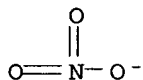
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:686594 CAPLUS

DOCUMENT NUMBER: 141:376571

TITLE: Phosphoprotein-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene

AUTHOR(S): Ojida, Akio; Kohira, Takahiro; Hamachi, Itaru  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Fukuoka, 812-8581, Japan

SOURCE: Chemistry Letters (2004), 33(8), 1024-1025  
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel **fluorescence** detection system using a chemosensor for **phosphoprotein** in gel electrophoresis anal. has been developed. The system employed bis-Zn(II)-dipicolylamine (Dpa)-appended anthracene as a **fluorescent** staining dye to carry out convenient and selective detection of **phosphoproteins** in SDS-PAGE.

CC 9-5 (Biochemical Methods)

ST **phosphoprotein** selective recognition **fluorescent** staining

IT Staining, biological  
(**fluorescent**; **phosphoprotein**-selective recognition)



and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **Fluorometry**

Gel electrophoresis

(**phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **Avidins**

Ovalbumin

**Phosphoproteins**

RL: ANT (Analyte); ANST (Analytical study)

(**phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **Albumins, analysis**

RL: ANT (Analyte); ANST (Analytical study)

(serum, bovine; **phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **Caseins, analysis**

RL: ANT (Analyte); ANST (Analytical study)

( $\alpha$ -; **phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT 9001-63-2, Lysozyme 9031-11-2,  $\beta$ -Galactosidase

RL: ANT (Analyte); ANST (Analytical study)

(**phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **439681-63-7**

RL: ARU (Analytical role, unclassified); ANST (Analytical study)

(**phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

IT **439681-63-7**

RL: ARU (Analytical role, unclassified); ANST (Analytical study)

(**phosphoprotein**-selective recognition and staining in SDS-PAGE by bis-Zn(II)-dipicolylamine-appended anthracene)

RN 439681-63-7 CAPLUS

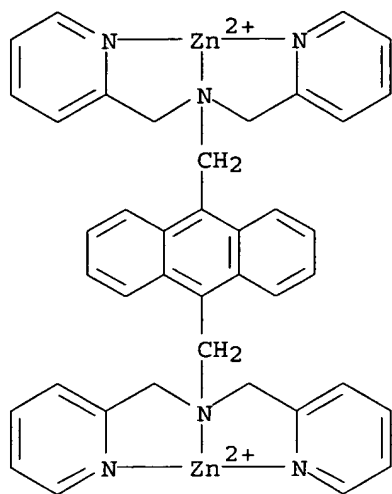
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

CM 1

CRN 360579-06-2

CMF C40 H36 N6 Zn2

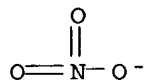
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER<sup>(5)</sup> OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:102814 CAPLUS

DOCUMENT NUMBER: 140:283712

TITLE: Molecular recognition and fluorescence sensing of **monophosphorylated** peptides in aqueous solution by bis(zinc(II)-dipicolylamine)-based artificial receptors

AUTHOR(S): Ojida, Akio; Mito-oka, Yasuko; Sada, Kazuki; Hamachi, Itaru

CORPORATE SOURCE: Graduate School of Engineering and Institute for Materials Chemistry and Engineering (IMCE), Department of Chemistry and Biochemistry, Kyushu University, Fukuoka, 812-8581, Japan

SOURCE: Journal of the American Chemical Society (2004), 126(8), 2454-2463

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The **phosphorylation** of proteins represents a ubiquitous mechanism for the cellular signal control of many different processes, and thus selective recognition and sensing of **phosphorylated** peptides and proteins in aqueous solution should be regarded as important targets

in the research field of mol. recognition. We now describe the design of **fluorescent** chemosensors bearing two zinc ions coordinated to distinct dipicolylamine (Dpa) sites. **Fluorescence** titration expts. show the selective and strong binding toward **phosphate** derivs. in aqueous solution. On the basis of <sup>1</sup>H NMR and <sup>31</sup>P NMR studies, and the single-crystal x-ray structural anal., it is clear that two Zn(Dpa) units of the binuclear receptors cooperatively act to bind a **phosphate** site of these derivs. Good agreement of the binding affinity estimated by isothermal titration calorimetry with **fluorescence** titration measurements revealed that these two receptors can **fluorometrically** sense several **phosphorylated** peptides that have consensus sequences modified with natural kinases. These chemosensors display the following significant features: (i) clear distinction between **phosphorylated** and **nonphosphorylated** peptides, (ii) sequence-dependent recognition, and (iii) strong binding to a neg. charged **phosphorylated** peptide, all of which can be mainly ascribed to coordination chemical and electrostatic interactions between the receptors and the corresponding peptides. Detailed titration expts. clarified that the **phosphate** anion-assisted coordination of the second Zn(II) to the binuclear receptors is crucial for the **fluorescence** intensification upon binding to the **phosphorylated** derivs. In addition, it is demonstrated that the binuclear receptors can be useful for the convenient **fluorescent** detection of a natural **phosphatase** (PTP1B) catalyzed **dephosphorylation**.

CC 9-5 (Biochemical Methods)

ST mol recognition **fluorescence** sensing **monophosphorylated** peptide

IT **Fluorometry**

Molecular modeling

Molecular recognition

(mol. recognition and **fluorescence** sensing of

**monophosphorylated** peptides in aqueous solution by

bis(zinc(II)-dipicolylamine)-based artificial receptors)

IT Titration

(thermometric; mol. recognition and **fluorescence** sensing of

**monophosphorylated** peptides in aqueous solution by

bis(zinc(II)-dipicolylamine)-based artificial receptors)

IT 56-65-5, Adenosine **triphosphate**, analysis 58-64-0, Adenosine

**diphosphate**, analysis 60-92-4, CAMP 61-19-8, Adenosine

**monophosphate**, analysis 512-56-1, Methyl **phosphate**

701-64-4, Phenyl **phosphate** 813-78-5, Dimethyl

**phosphate** 7558-80-7, Sodium dihydrogen **phosphate**

21820-51-9, O-**Phospho**-L-tyrosine 300865-11-6, PTP-1B

439681-10-4 439681-11-5 439681-12-6 439681-13-7 676145-48-5

676145-49-6 676145-50-9

RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); ANST (Analytical study); PROC (Process)

(mol. recognition and **fluorescence** sensing of

**monophosphorylated** peptides in aqueous solution by

bis(zinc(II)-dipicolylamine)-based artificial receptors)

IT 439681-63-7P 439681-65-9P 439681-67-1P 676257-32-2P

676257-34-4P

RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process)

(mol. recognition and **fluorescence** sensing of

**monophosphorylated** peptides in aqueous solution by

bis(zinc(II)-dipicolylamine)-based artificial receptors)

IT 439681-63-7P 439681-65-9P

RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process)  
 (mol. recognition and **fluorescence** sensing of  
**monophosphorylated** peptides in aqueous solution by  
 bis(zinc(II)-dipicolylamine)-based artificial receptors)

RN 439681-63-7 CAPLUS

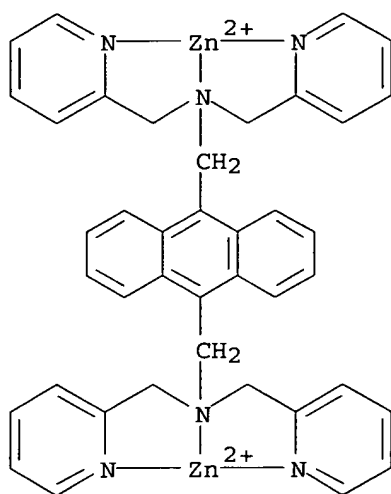
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

CM 1

CRN 360579-06-2

CMF C40 H36 N6 Zn2

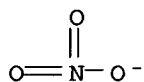
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



RN 439681-65-9 CAPLUS

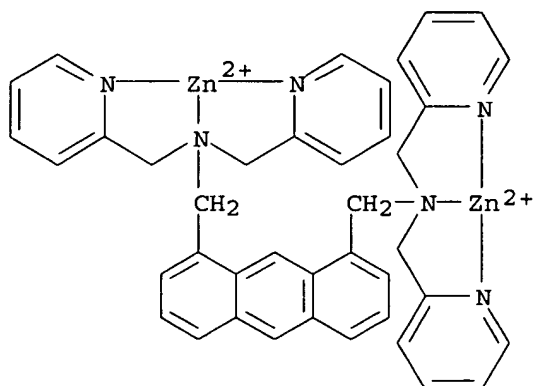
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-1,8-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

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CRN 439681-64-8

CMF C40 H36 N6 Zn2

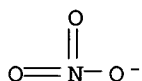
CCI CCS



CM 2

CRN 14797-55-8

CMF N 03



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:817127 CAPLUS

DOCUMENT NUMBER: 140:12086

TITLE: Crystal structures of 9,10-bis[bis(2-pyridylmethyl)aminomethyl]anthracene and its ZnCl<sub>2</sub> complex. Intramolecular  $\pi$ - $\pi$  interaction between anthracene and ZnCl<sub>2</sub>-complexed pyridine

AUTHOR(S): Kubo, Kanji; Mori, Akira

CORPORATE SOURCE: Institute for Materials Chemistry and Engineering, Kyushu University, Kasuga, 816-8580, Japan

SOURCE: Chemistry Letters (2003), 32(10), 926-927

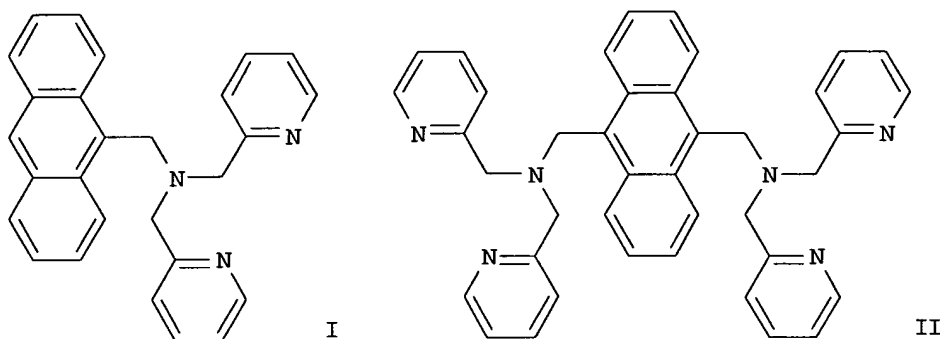
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



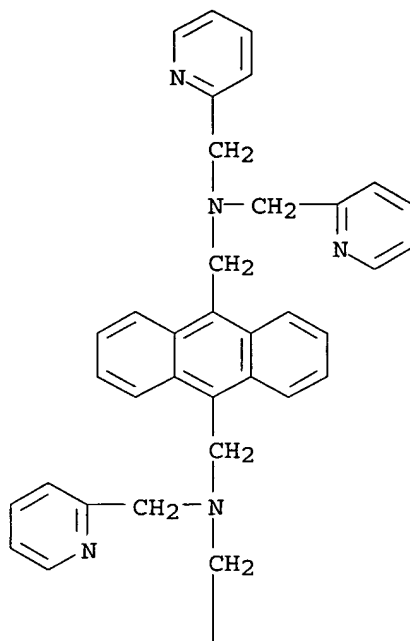
- AB Anthracene derivs. having dipicolylaminomethyl group (I and II) exhibited an emission-intensity enhancement in the presence of  $Zn^{2+}$ . From an x-ray crystallog. anal. of II and  $II \cdot 2ZnCl_2$ , the binding of  $Zn^{2+}$  to the dipicolylaminomethyl unit inhibits the photoinduced electron transfer process. Intramol.  $\pi$ - $\pi$  interactions between the anthracene and the  $ZnCl_2$ -complexed pyridine were observed
- CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 73, 75
- ST zinc pyridylmethylaminomethylanthracene prepn structure  
**fluorescence** enhancement; crystal structure  
pyridylmethylaminomethylanthracene zinc chloro
- IT **Fluorescence**  
Pi-pi interaction  
(**fluorescence** enhancement in zinc bis[bis(pyridylmethyl)aminomethyl]anthracene complex due to inhibition of photoinduced electron transfer and generation of intramol. anthracene-pyridine pi-pi interactions)
- IT Electron transfer  
(intramol., photochem.; **fluorescence** enhancement in zinc bis[bis(pyridylmethyl)aminomethyl]anthracene complex due to inhibition of photoinduced electron transfer and generation of intramol. anthracene-pyridine pi-pi interactions)
- IT **628297-13-2**  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(crystal structure and **fluorescence** enhancement by complexation with zinc)
- IT 190183-94-9  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(**fluorescence** enhancement by complexation with zinc)
- IT **628297-14-3P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and **fluorescence** enhancement in zinc [bis(pyridylmethyl)aminomethyl]anthracene complex due to inhibition of photoinduced electron transfer and generation of intramol. anthracene-pyridine pi-pi interactions)
- IT **628297-15-4P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, crystal structure and **fluorescence** enhancement in zinc [bis(pyridylmethyl)aminomethyl]anthracene complex due to inhibition of photoinduced electron transfer and generation of intramol. anthracene-pyridine pi-pi interactions)
- IT **628297-13-2**  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(crystal structure and **fluorescence** enhancement by

complexation with zinc)

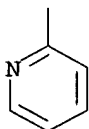
RN 628297-13-2 CAPLUS

CN 9,10-Anthracenedimethanamine, N,N,N',N'-tetrakis(2-pyridinylmethyl) - (9CI)  
(CA INDEX NAME)

PAGE 1-A



PAGE 2-A



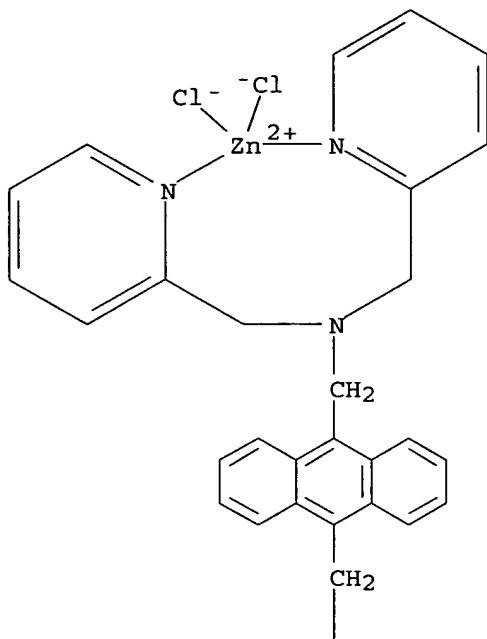
IT 628297-15-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, crystal structure and **fluorescence** enhancement in  
 zinc [bis(pyridylmethyl)aminomethyl]anthracene complex due to  
 inhibition of photoinduced electron transfer and generation of  
 intramol. anthracene-pyridine pi-pi interactions)

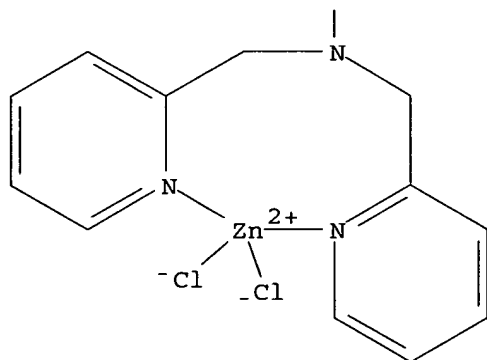
RN 628297-15-4 CAPLUS

CN Zinc, tetrachloro[μ-[N,N,N',N'-tetrakis[(2-pyridinyl-κN)methyl] -  
9,10-anthracenediamine]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:679068 CAPLUS

DOCUMENT NUMBER: 139:210392

TITLE: **Fluorescence sensor for phosphate ion and phosphorylated peptide**

INVENTOR(S): Hamachi, Itaru

PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan

SOURCE: PCT Int. Appl., 22 pp.

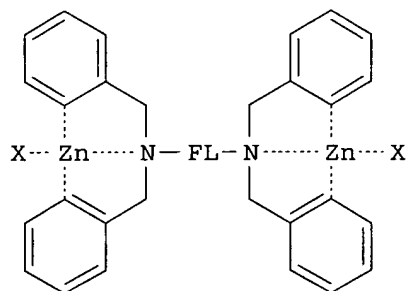
CODEN: PIXXD2

DOCUMENT TYPE: Patent



LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.  | KIND | DATE              | APPLICATION NO. | DATE       |
|---|------|-------------------|-----------------|------------|
| <del>WO 2003071280</del>  | A1   | 20030828          | WO 2003-JP705   | 20030127   |
| W: US   |      |                   |                 |            |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR    |      |                   |                 |            |
| JP 2003246788   | A2   | 20030902          | JP 2002-45846   | 20020222   |
| EP 1484614  | A1   | 20041208          | EP 2003-742658  | 20030127   |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, HU, SK |      |                   |                 |            |
| US 2005148086   | A1   | 20050707          | US 2003-505056  | 20030127   |
| PRIORITY APPLN. INFO.:  |      |                   | JP 2002-45846   | A 20020222 |
|   |      |                   | WO 2003-JP705   | W 20030127 |
| OTHER SOURCE(S):  |      | MARPAT 139:210392 |                 |            |
| GI  |      |                   |                 |            |



I

AB A fluorescence sensor for detecting **phosphate** ions or **phosphorylated** peptides with high sensitivity is disclosed, which comprises a compound (zinc dipicolylamine binuclear complex) selectively **fluorescent** by the action of **phosphate** ions and represented by the following general formula (I). In the formula I, FL represents a **fluorescent** functional group or atomic group which has an aromatic ring or heterocycle (e.g., dimethylanthyryl), and X represents a functional group or atomic group which undergoes elimination in an aqueous solution to become an anion (e.g., NO<sub>3</sub>). Zn(Dpa)-9,10-Anth complex was shown to exhibit a strong **fluorescence** selectively with **phosphate** ion or with a peptide possessing a **phosphorylated** amino acid as well as hydrophobic amino acid(s) and neg. charged amino acid(s).

IC ICM G01N033-58  
 ICS G01N033-52; G01N021-78; G01N021-77; C07D213-36; C09K011-06

CC 9-5 (Biochemical Methods)

ST **fluorescence** sensor **phosphate** ion  
**phosphorylated** peptide

IT **Fluorescent** substances  
 (fluorescence sensor for **phosphate** ion and  
**phosphorylated** peptide)

IT Sensors  
 (fluorometric; fluorescence sensor for  
**phosphate** ion and **phosphorylated** peptide)

IT Peptides, analysis

RL: ANT (Analyte); ANST (Analytical study)  
 (phosphorylated; fluorescence sensor for  
 phosphate ion and phosphorylated peptide)

IT 14265-44-2, Phosphate, analysis  
 RL: ANT (Analyte); ANST (Analytical study)  
 (fluorescence sensor for phosphate ion and  
 phosphorylated peptide)

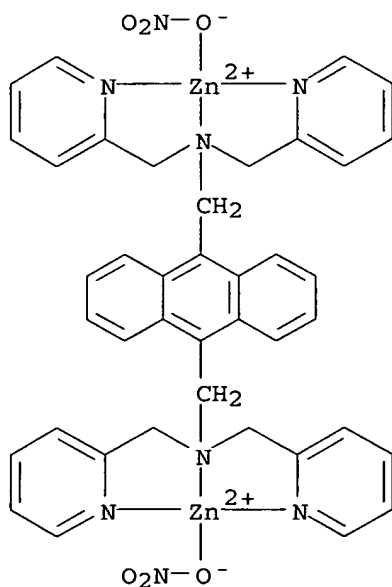
IT 389142-16-9P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation); USES (Uses)  
 (fluorescence sensor for phosphate ion and  
 phosphorylated peptide)

IT 7779-88-6, Zinc nitrate 10387-13-0, 9,10-Bis(chloromethyl)anthracene  
 29227-68-7, Dipicolylamine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (fluorescence sensor for phosphate ion and  
 phosphorylated peptide)

IT 389142-16-9P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation); USES (Uses)  
 (fluorescence sensor for phosphate ion and  
 phosphorylated peptide)

RN 389142-16-9 CAPLUS

CN Zinc(2+), bis(nitrato-κO) [μ-[N,N,N',N'-tetrakis[(2-pyridinyl-  
 κN)methyl]-9,10-anthracenedimethanamine-κN:κN']]di-  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:586198 CAPLUS

DOCUMENT NUMBER: 137:332557

TITLE: Efficient fluorescent ATP-sensing based on coordination chemistry under aqueous neutral conditions

AUTHOR(S): Ojida, Akio; Park, Sun-kyu; Mito-oka, Yasuko; Hamachi, Itaru

CORPORATE SOURCE: PRESTO (Organization and Function, JST), Kyushu University, Fukuoka, 812-8581, Japan

SOURCE: Tetrahedron Letters (2002), 43(35), 6193-6195  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new **fluorescent** chemosensor consisting of zinc-dipicolylamine appended anthracene for ATP which can efficiently act in neutral aqueous solution, was developed.

CC 80-2 (Organic Analytical Chemistry)

ST ATP **fluorescence** sensor zinc dipicolylamine appended anthracene reagent

IT Optical sensors  
(**fluorescent** chemosensor consisting of zinc-dipicolylamine appended anthracene for ATP)

IT Anions  
(**fluorescent** response of zinc-dipicolylamine appended anthracene to)

IT **Fluorescence**  
(of zinc-dipicolylamine appended anthracene for ATP sensing)

IT 56-65-5, ATP, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(**fluorescent** chemosensor consisting of zinc-dipicolylamine appended anthracene for ATP)

IT **473773-72-7P**  
RL: ARU (Analytical role, unclassified); DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(**fluorescent** chemosensor consisting of zinc-dipicolylamine appended anthracene for ATP)

IT 58-64-0, ADP, analysis 61-19-8, AMP, analysis  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(**fluorescent** response and association of zinc-dipicolylamine appended anthracene to)

IT 65-47-4, CTP 71-50-1, Acetate, analysis 86-01-1, GTP 812-00-0, **Monomethylphosphate** 813-78-5, **Dimethylphosphate** 3812-32-6, Carbonate, analysis 14265-44-2, **Phosphate**, analysis 14343-69-2, Azide 14797-55-8, Nitrate, analysis 14808-79-8, Sulfate, analysis 16887-00-6, Chloride, analysis  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(**fluorescent** response of zinc-dipicolylamine appended anthracene to)

IT 1539-42-0, 2,2'-Dipicolylamine 7779-88-6, Zinc nitrate 473773-73-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(in preparation of zinc-dipicolylamine appended anthracene for **fluorescent** ATP-sensing)

IT 473773-74-9P 473773-75-0P **473773-76-1P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(in preparation of zinc-dipicolylamine appended anthracene for **fluorescent** ATP-sensing)

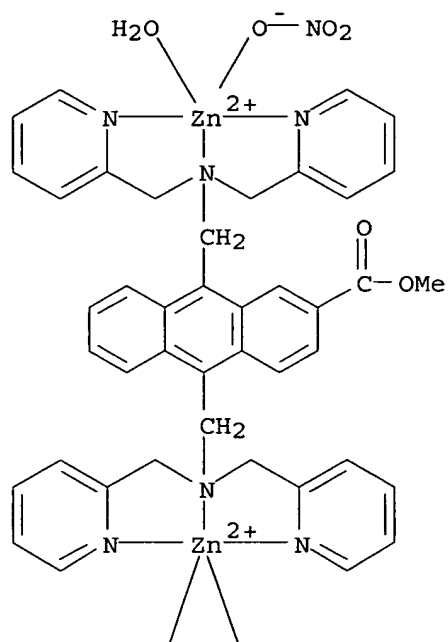
IT **473773-72-7P**  
RL: ARU (Analytical role, unclassified); DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(**fluorescent** chemosensor consisting of zinc-dipicolylamine appended anthracene for ATP)

RN 473773-72-7 CAPLUS  
 CN Zinc(2+), diaqua[μ-[methyl 9,10-bis[[[(2-pyridinyl-κN)methyl]amino-κN]methyl]-2-anthracenecarboxylate]]bis(nitrate-κO)di-, dinitrate (9CI) (CA INDEX NAME)

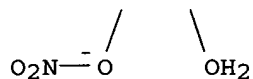
CM 1

CRN 473773-71-6  
 CMF C42 H42 N8 O10 Zn2  
 CCI CCS

PAGE 1-A

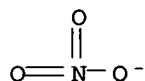


PAGE 2-A



CM 2

CRN 14797-55-8  
 CMF N O3



IT 473773-76-1P

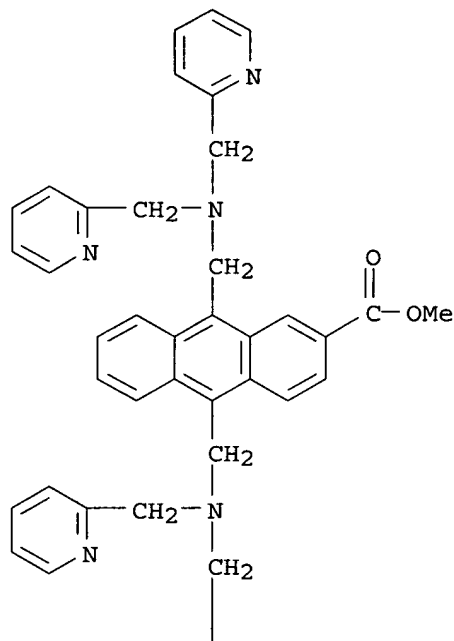
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of zinc-dipicolylamine appended anthracene for fluorescent ATP-sensing)

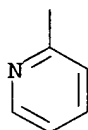
RN 473773-76-1 CAPLUS

CN 2-Anthracenecarboxylic acid, 9,10-bis[[bis(2-pyridinylmethyl)amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:344031 CAPLUS

DOCUMENT NUMBER: 137:59821

TITLE: First artificial receptors and chemosensors toward phosphorylated peptide in aqueous solution

AUTHOR(S): Ojida, Akio; Mitooka, Yasuko; Inoue, Masaaki; Hamachi, Itaru

CORPORATE SOURCE: PRESTO (Organization and Function JST) Institute for Fundamental Research of Organic Chemistry (IFOC)

Department of Chemistry and Biochemistry Graduate  
School of Engineering, Kyushu University, Fukuoka,  
812-8581, Japan

SOURCE: Journal of the American Chemical Society (2002),  
124(22), 6256-6258  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The first **fluorescent** chemosensors toward a native  
**phosphorylated** peptide are successfully synthesized. Dinuclear  
zinc(II)-dipicolylamine-based anthracene (1, 2) can selectively recognize  
and sense **phosphorylated** species with an increase in the  
**fluorescence** intensity. We also demonstrated that these  
artificial receptors **fluorometrically** detect a  
**phosphorylated** peptide with high affinity (>10<sup>7</sup> M<sup>-1</sup>) in aqueous solution

CC 9-16 (Biochemical Methods)

ST artificial receptor chemosensor **phosphorylation** peptide aq soln

IT **Fluorometry**  
Molecular association  
Molecular recognition  
**Phosphorylation**, biological  
Sensors  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

IT Peptides, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

IT Receptors  
RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or  
chemical process); PYP (Physical process); ANST (Analytical study); PROC  
(Process)  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

IT 439681-10-4 439681-11-5 439681-12-6 439681-13-7  
RL: ANT (Analyte); ANST (Analytical study)  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

IT 21820-51-9 439681-63-7 439681-65-9 439681-67-1  
RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or  
chemical process); PYP (Physical process); ANST (Analytical study); PROC  
(Process)  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

IT 439681-63-7 439681-65-9  
RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or  
chemical process); PYP (Physical process); ANST (Analytical study); PROC  
(Process)  
(artificial receptors and chemosensors toward **phosphorylated**  
peptide in aqueous solution)

RN 439681-63-7 CAPLUS

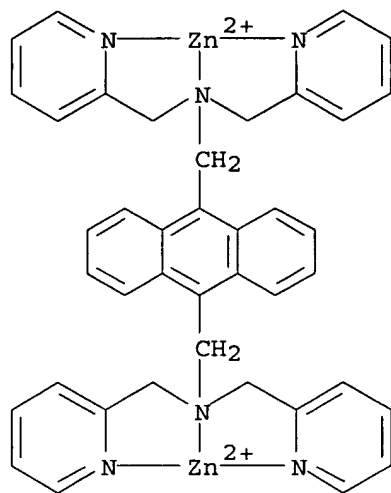
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-  
anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA  
INDEX NAME)

CM 1

CRN 360579-06-2

CMF C40 H36 N6 Zn2

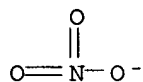
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



RN 439681-65-9 CAPLUS

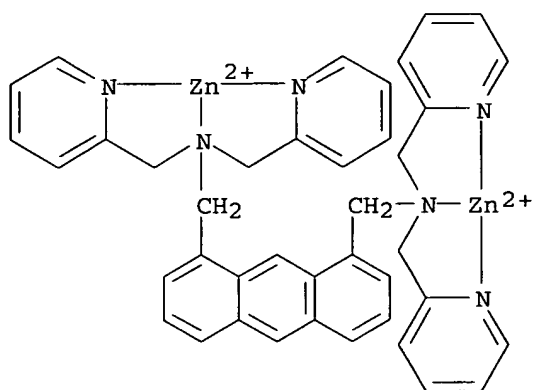
CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-1,8-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, tetranitrate (9CI) (CA INDEX NAME)

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CRN 439681-64-8

CMF C40 H36 N6 Zn2

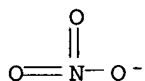
CCI CCS



CM 2

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L77 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:683996 CAPLUS

DOCUMENT NUMBER: 135:242147

TITLE: Preparation of 2,2'-dipicolylamine zinc complexes as receptors for proteins and peptides.

INVENTOR(S): Hamaji, Itaru

PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

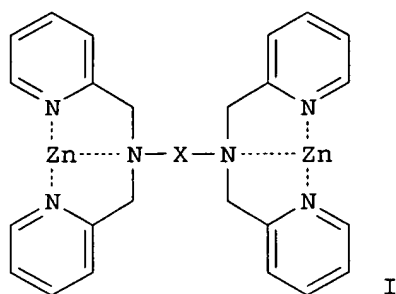
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND   | DATE       | APPLICATION NO. | DATE     |
|------------------------|--------|------------|-----------------|----------|
| -----                  | ---    | -----      | -----           | -----    |
| JP 2001253871          | A2     | 20010918   | JP 2000-66132   | 20000310 |
| PRIORITY APPLN. INFO.: |        |            | JP 2000-66132   | 20000310 |
| OTHER SOURCE(S):       | MARPAT | 135:242147 |                 |          |
| GI                     |        |            |                 |          |





AB The receptors I (X = aromatic or heterocyclic ring having 2 methylene groups as the side chain, e.g. CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, etc.), useful as tools for biochem. researches, etc., are claimed. I (X = p-CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>) (preparation given) was treated with Ac-Ala-Glu-Ala-Ala-Lys-Glu-Ala-His-Ala-Lys-Glu-Ala-Ala-Ala-His-Ala-NH<sub>2</sub> in a borate buffer to induce α-helix structure.

IC ICM C07D213-36

ICS G01N033-566; C07K007-08

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 6

IT 360579-06-2

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(preparation of binuclear 2,2'-dipicolylamine zinc complexes as receptors for proteins and peptides)

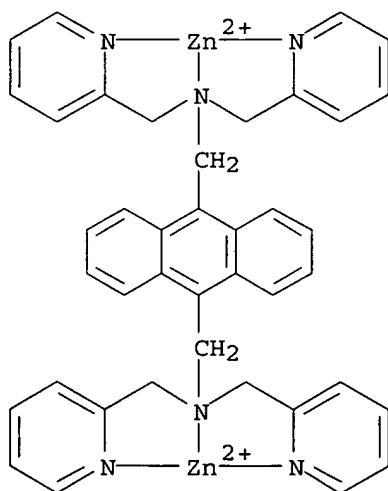
IT 360579-06-2

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(preparation of binuclear 2,2'-dipicolylamine zinc complexes as receptors for proteins and peptides)

RN 360579-06-2 CAPLUS

CN Zinc(4+), [μ-[N,N,N',N'-tetrakis[(2-pyridinyl-κN)methyl]-9,10-anthracenedimethanamine-κN:κN']]di- (9CI) (CA INDEX NAME)

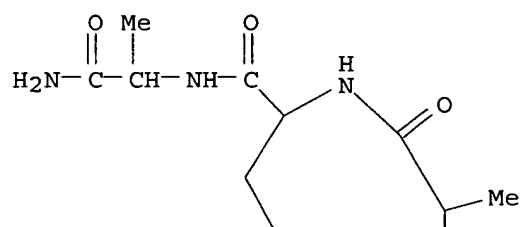


L77 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

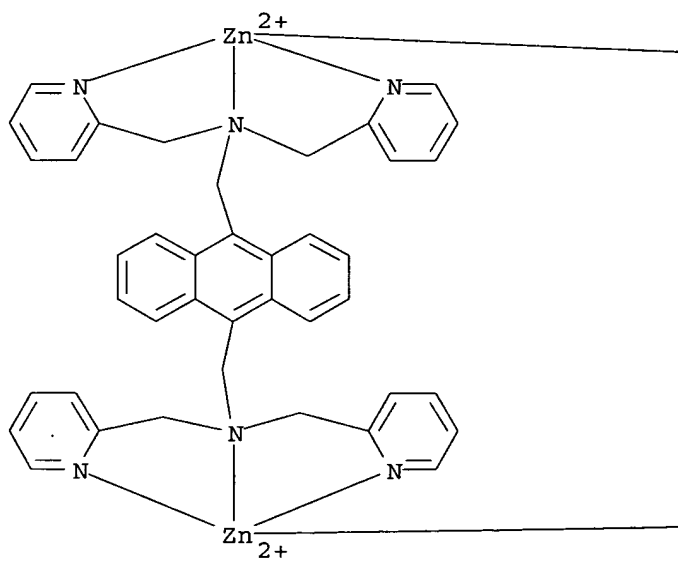
ACCESSION NUMBER: 2001:674575 CAPLUS  
 DOCUMENT NUMBER: 136:102633  
 TITLE: Zn(II) dipicolylamine-based artificial receptor as a new entry for surface recognition of  $\alpha$ -helical peptides in aqueous solution  
 AUTHOR(S): Mito-Oka, Y.; Tsukiji, S.; Hiraoka, T.; Kasagi, N.; Shinkai, S.; Hamachi, I.  
 CORPORATE SOURCE: Graduate School of Engineering, Department of Chemistry and Biochemistry, Kyushu University, Fukuoka, 812-8581, Japan  
 SOURCE: Tetrahedron Letters (2001), 42(40), 7059-7062  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB It is clear by CD spectral titration that Zn(II)dipicolylamine-based dinuclear complexes selectively bind and ~~stabilize the  $\alpha$ -helix conformation of peptides having two histidine (His) residues~~ at specific positions (H-i and i+4 or i+7 or i+11).  
 CC 34-3 (Amino Acids, Peptides, and Proteins)  
 Section cross-reference(s): 22, 78  
 IT 389142-19-2 389142-20-5 389142-21-6 389142-22-7  
 389142-23-8  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (binding consts. of helical peptides by Zn(II) dipicolylamine-based artificial receptor in aqueous solution)  
 IT 389142-16-9P 389142-17-0P 389142-18-1P 389142-24-9P  
 389142-25-0P 389142-26-1P 389142-27-2P  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation of Zn(II) complexes of dipicolylamine derivs. as artificial receptors for helical histidine peptides)  
 IT 389142-19-2 389142-20-5  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (binding consts. of helical peptides by Zn(II) dipicolylamine-based artificial receptor in aqueous solution)  
 RN 389142-19-2 CAPLUS  
 CN Zinc(2+), [ $\mu$ -[N-acetyl-L-alanyl-L- $\alpha$ -glutamyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L- $\alpha$ -glutamyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-histidyl- $\kappa$ N1-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-histidyl- $\kappa$ N1-L-alaninamidato(2-)]][ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl]-9,10-anthracenedimethanamine- $\kappa$ N: $\kappa$ N']]di-, dihydrogen (9CI)  
 (CA INDEX NAME)

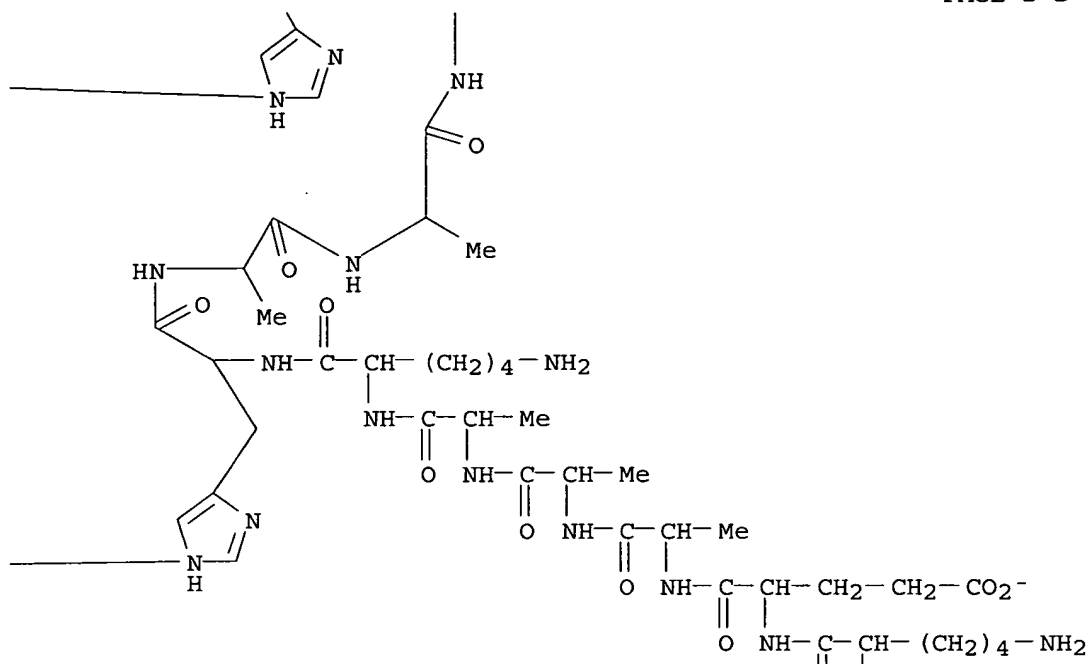
PAGE 1-B



PAGE 2-A



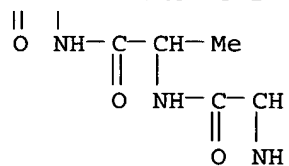
PAGE 2-B



PAGE 3-A

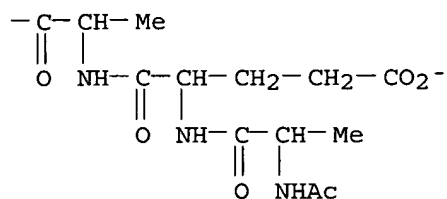
● 2 H<sup>+</sup>

PAGE 3-B



PAGE 3-C

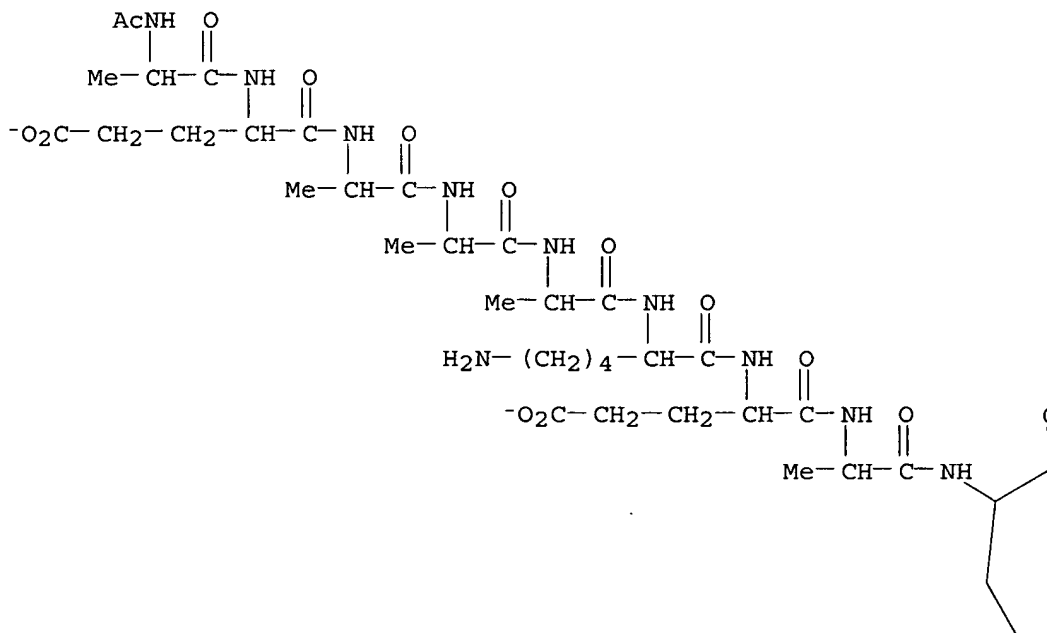
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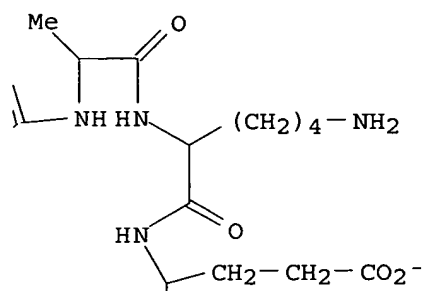
RN 389142-20-5 CAPLUS

CN Zinc(1+), [μ-[N-acetyl-L-alanyl-L-α-glutamyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-α-glutamyl-L-alanyl-L-histidyl-κN1-L-alanyl-L-lysyl-L-α-glutamyl-L-alanyl-L-alanyl-L-alanyl-L-histidyl-κN1-L-alaninamidato(3-)] [μ-[N,N,N',N'-tetrakis[(2-pyridinyl-κN)methyl]-9,10-anthracenedimethanamine-κN:κN']]di-, trihydrogen (9CI)  
(CA INDEX NAME)

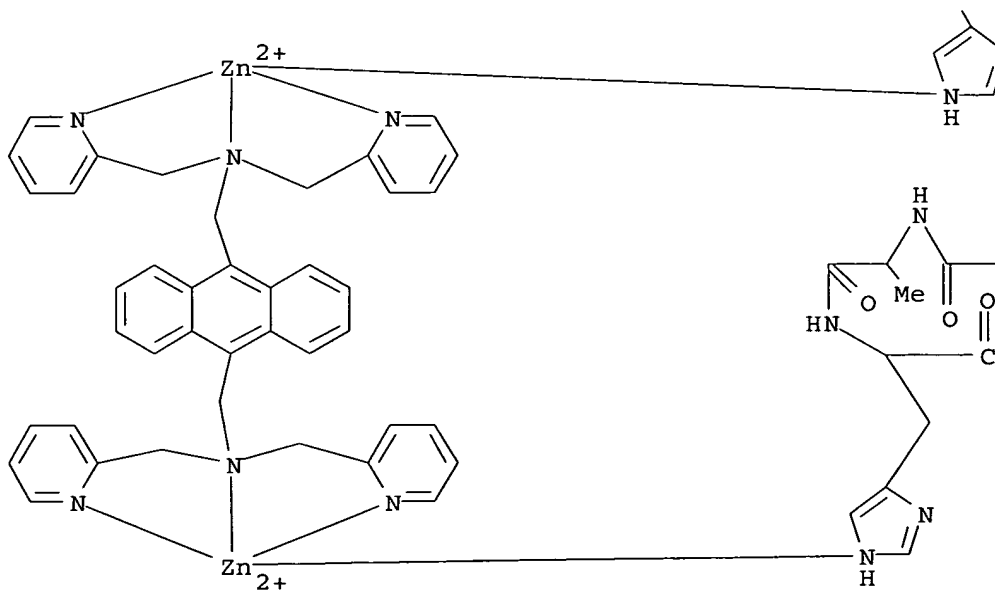
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PAGE 1-B



PAGE 2-A

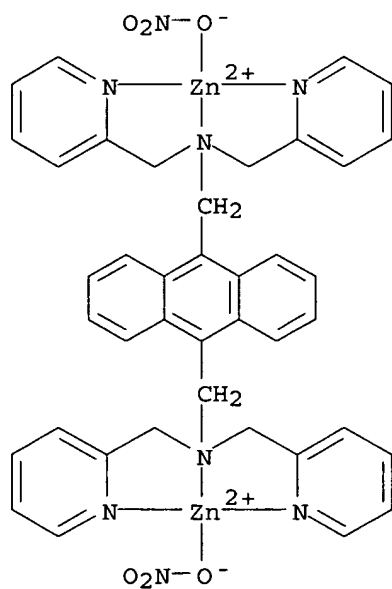


CC(C)NC(=O)N1C(=O)C(C)CC1C(=O)NC(=O)N $\bullet_3 \text{H}^+$ 

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

RN 389142-16-9 CAPLUS

CN    Zinc(2+), bis(nitrato-κO) [μ-[N,N,N',N'-tetrakis[(2-pyridinyl-κN)methyl]-9,10-anthracenedimethanamine-κN:κN']] di-(9CI)    (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DICTIONARY FILE UPDATES: 26 MAR 2006 HIGHEST RN 878044-67-8

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* available and contains the CA role and document type information. *
*
*****
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FILE LAST UPDATED: 26 Mar 2006 (20060326/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE



=&gt; d que nos L38

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L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L25         29863 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?SPHING?/BI
L38         0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L25

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=&gt; d que nos L39

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L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L21         2046864 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSP?/BI
L23         1420774 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?FLUOR?/BI
L36         66 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L21
L37         96 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L23
L39         37 SEA FILE=CAPLUS ABB=ON  PLU=ON  L36 AND L37

```

=&gt; d que nos L41

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L40         228358 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSPHATID?/BI OR ?PHOSPHOLIP?
L41         5 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L40

```

=&gt; d que nos L42

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L23         1420774 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?FLUOR?/BI
L40         228358 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSPHATID?/BI OR ?PHOSPHOLIP?
L41         5 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L40
L42         4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L41 AND L23

```

=&gt; d que nos L45

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L21         2046864 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSP?/BI
L43         466 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND (CU>0 OR NI>0 OR
L44         133 SEA FILE=CAPLUS ABB=ON  PLU=ON  L43
L45         21 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44 AND L21

```

=&gt; d que nos L53

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L21         2046864 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSP?/BI
L23         1420774 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?FLUOR?/BI
L43         466 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND (CU>0 OR NI>0 OR
L44         133 SEA FILE=CAPLUS ABB=ON  PLU=ON  L43
L45         21 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44 AND L21
L46         40 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44 AND L23
L53         12 SEA FILE=CAPLUS ABB=ON  PLU=ON  L45 AND L46

```

=&gt; d que nos L65

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L43         466 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND (CU>0 OR NI>0 OR
              CO>0 OR EU>0 OR NB>0)
L44         133 SEA FILE=CAPLUS ABB=ON  PLU=ON  L43
L64         440778 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?LIPID?/BI
L65         1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44 AND L64

```

=&gt; d que nos L66

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L64         440778 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?LIPID?/BI
L66         4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L64

```

=&gt; d que nos L68

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L67         149726 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?SERIN?/BI
L68         7 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L67

```

=&gt; d que nos L70

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L23         1420774 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?FLUOR?/BI
L43         466 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND (CU>0 OR NI>0 OR
              CO>0 OR EU>0 OR NB>0)
L44         133 SEA FILE=CAPLUS ABB=ON  PLU=ON  L43
L46         40 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44 AND L23
L69         QUE ABB=ON  PLU=ON  ?CELL?/BI OR ?VESICL?/BI
L70         4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L69 AND L46

```

=&gt; d que nos L74

```

L7          STR
L11         1261 SEA FILE=REGISTRY SSS FUL L7
L13         330 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L21         2046864 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?PHOSP?/BI
L23         1420774 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?FLUOR?/BI
L25         29863 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?SPHING?/BI
L64         440778 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?LIPID?/BI
L69         QUE ABB=ON  PLU=ON  ?CELL?/BI OR ?VESICL?/BI
L71         39 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 AND L69
L74         24 SEA FILE=CAPLUS ABB=ON  PLU=ON  L71 AND (L21 OR L23 OR L25 OR
              L64)

```

```

=> s L38 or L39 or L41 or L42 or L45 or L53 or L65 or L66 or L68 or L70 or L74
L78         64 L38 OR L39 OR L41 OR L42 OR L45 OR L53 OR L65 OR L66 OR L68 OR
              L70 OR L74

```

=&gt; s L78 not (L58 or L77)

```

L79         52 L78 NOT (L58 OR L77)

```

=&gt; d ibib abs hitind hitstr L79 1-52

L79 ANSWER (1) OF 52 CAPLUS (COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:116625 CAPLUS

DOCUMENT NUMBER: 144:187554

TITLE: Generic probes for the detection of phosphorylated sequences

INVENTOR(S): Morgenstern, Kurt A.; Boyce, Jim; Chipman, Stewart

PATENT ASSIGNEE(S): Amgen Inc., USA

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| WO 2006014645   | A1   | 20060209 | WO 2005-US25587 | 20050720 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,<br>CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,<br>LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,<br>NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,<br>SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,<br>ZA, ZM, ZW<br>RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,<br>IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,<br>CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,<br>GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,<br>KG, KZ, MD, RU, TJ, TM |      |          |                 |          |

PRIORITY APPLN. INFO.: US 2004-590705P P 20040723

AB Generic probes that bind to **phosphorylated** amino acid residues are provided as well as methods employing the probes for screening for kinase inhibitory activity, kinase activity, and **phosphatase** activity. A variety of compds. containing a coupling group, chelating group and a linker are claimed. Methods for distinguishing **serine** /threonine kinase **phosphorylation** from tyrosine kinase **phosphorylation** are also provided.

IC ICM C07D401-14

ICS A61K031-44; A61K031-47

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 7, 78

ST **fluorescent** probe **phosphorylated** amino acid residue;  
**serine** threonine kinase **phosphorylation**  
**fluorescent** probe; tyrosine kinase **phosphorylation**  
**fluorescent** probe; protein kinase activity **fluorescent**  
 probe; lanthanide complex **fluorescent** probe  
**phosphorylated** sequence

IT **Fluorescence** resonance energy transfer

Fluorescent indicators

Phosphorylation, biological

(fluorescent probes for detection of **phosphorylated** sequences and screening kinase **phosphorylation**)IT **Phosphopeptides**

Phosphoproteins

RL: ANT (Analyte); ANST (Analytical study)

(fluorescent probes for detection of **phosphorylated** sequences and screening kinase **phosphorylation**)

IT Rare earth complexes  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 9026-43-1 80449-02-1  
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
 study); BIOL (Biological study)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 151175-68-7 167962-83-6 167962-85-8 875057-37-7  
 875057-38-8 875057-39-9 875057-41-3 875057-42-4  
 875057-45-7 875057-46-8  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 875057-34-4P 875057-35-5P  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL  
 (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES  
 (Uses)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 875057-44-6P  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological  
 study); PREP (Preparation); USES (Uses)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

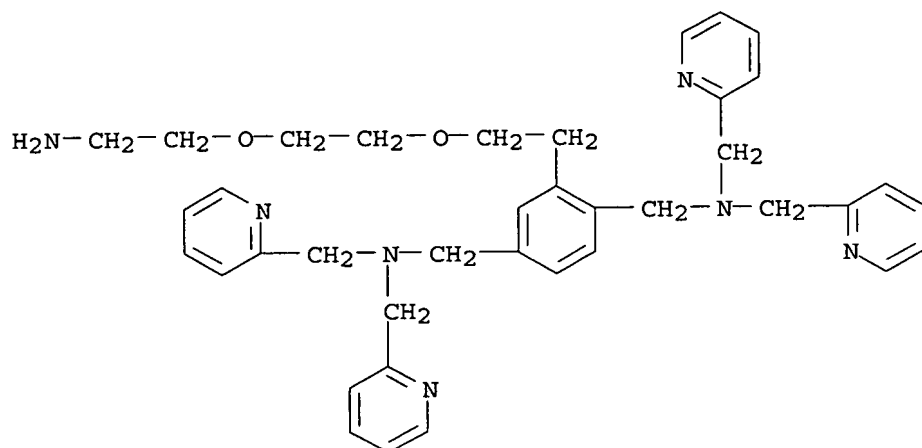
IT 929-59-9 5437-45-6, Benzyl 2-bromoacetate 153086-78-3 391624-47-8  
 875057-43-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 875057-36-6P 875057-40-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

IT 875057-37-7 875057-38-8  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (fluorescent probes for detection of phosphorylated  
 sequences and screening kinase phosphorylation)

RN 875057-37-7 CAPLUS

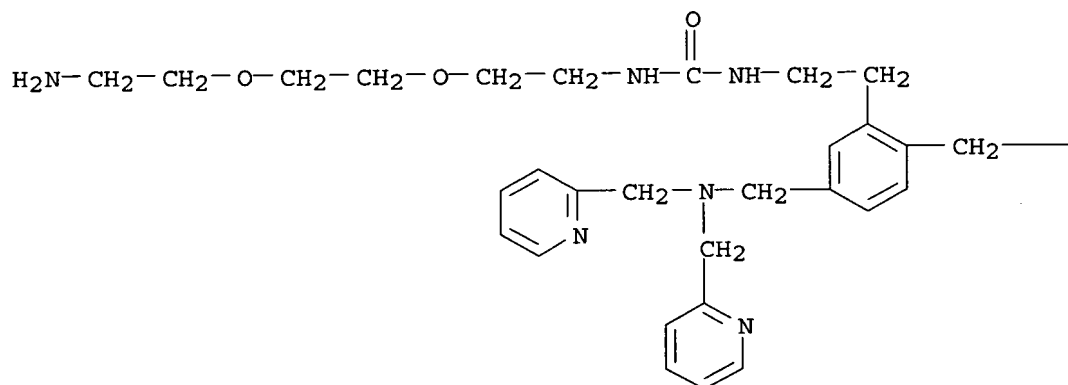
CN 1,4-Benzenedimethanamine, 2-[2-[2-(2-aminoethoxy)ethoxy]ethyl]-N,N,N',N'-  
 tetrakis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



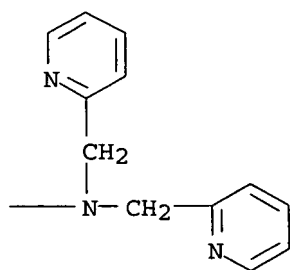
RN 875057-38-8 CAPLUS

CN Urea, N-[2-[2-(2-aminoethoxy)ethoxy]ethyl]-N'-[2-[2,5-bis[[bis(2-pyridinylmethyl)amino]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 2 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:68197 CAPLUS

DOCUMENT NUMBER: 144:249908

TITLE: 6-Methylpyridyl for Pyridyl Substitution Tunes the  
Properties of **Fluorescent** Zinc Sensors of  
the Zinpyr Family

AUTHOR(S): Goldsmith, Christian R.; Lippard, Stephen J.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of  
Technology, Cambridge, MA, 02139, USA

SOURCE: Inorganic Chemistry (2006), 45(2), 555-561

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To prepare **fluorescent** zinc sensors with binding affinities lower  
than that of the parent 9-(o-carboxyphenyl)-2,7-dichloro-4,5-bis(bis(2-  
pyridylmethyl)methylaminomethyl)-6-hydroxy-3-xanthenone (ZP1),  
dimethylated and tetramethylated derivs. were synthesized having either  
two or four of the pyridyl subunits methylated at the 6-position. Like  
the parent ZP1, both Me2ZP1 and Me4ZP1 exhibit increased  
**fluorescence** in the presence of Zn<sup>2+</sup>. The integrated emission of  
Me2ZP1 increases 4-fold in the presence of excess zinc, whereas Me4ZP1  
displays 2.5-fold enhanced **fluorescence** for Zn<sup>2+</sup>. Methylating  
the 6-positions of the pyridyl rings raises the dissociation constant of the  
sensors and lowers the pKa values associated with the tertiary amine ligands  
in a systematic manner. The properties of the dimethylated Me2ZP1 dye  
resemble those of ZP1, but the tetramethylated Me4ZP1 differs greatly from  
ZP1 in terms of its brightness, affinity toward Zn<sup>2+</sup>, exchange kinetics,  
and metal sensitivity. Both Me2ZP1 and Me4ZP1 can enter HeLa  
cells and signal the presence of Zn<sup>2+</sup>. Staining caused by both  
dyes is punctate, with localization patterns resembling that observed for  
ZP1.

CC 9-16 (Biochemical Methods)

Section cross-reference(s): 29

ST methylpyridyl pyridyl **fluorescent** probe zinc zinpyr

IT Imaging

(**fluorescent**; preparation, chemical photophys., and Zn-responsive  
**fluorescence** properties of methylated derivs. of zinpyr ZP 1  
zinc sensor)

IT **Fluorescence**

**Fluorescence** microscopy

Human

Methyl group

Molecular association

Staining, biological

(preparation, chemical photophys., and Zn-responsive **fluorescence**  
properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

IT **Fluorescent** indicators

(zinc sensor; preparation, chemical photophys., and Zn-responsive  
**fluorescence** properties of methylated derivs. of zinpyr ZP 1  
zinc sensor)

IT 7440-66-6, Zinc, analysis

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
study); BIOL (Biological study)

(preparation, chemical photophys., and Zn-responsive **fluorescence**  
properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

IT 288574-78-7

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(preparation, chemical photophys., and Zn-responsive **fluorescence** properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

IT **877375-13-8P 877375-14-9P**

RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, chemical photophys., and Zn-responsive **fluorescence** properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

IT 25599-07-9, Bis(6-methyl-2-pyridylmethyl)amine 30525-89-4, Paraformaldehyde 210175-88-5, (2-Pyridylmethyl)(6-methyl-2-pyridylmethyl)amine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation, chemical photophys., and Zn-responsive **fluorescence** properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

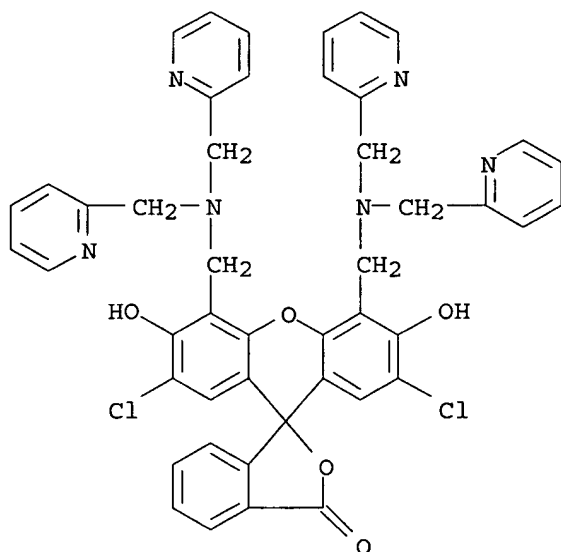
IT **288574-78-7**

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(preparation, chemical photophys., and Zn-responsive **fluorescence** properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



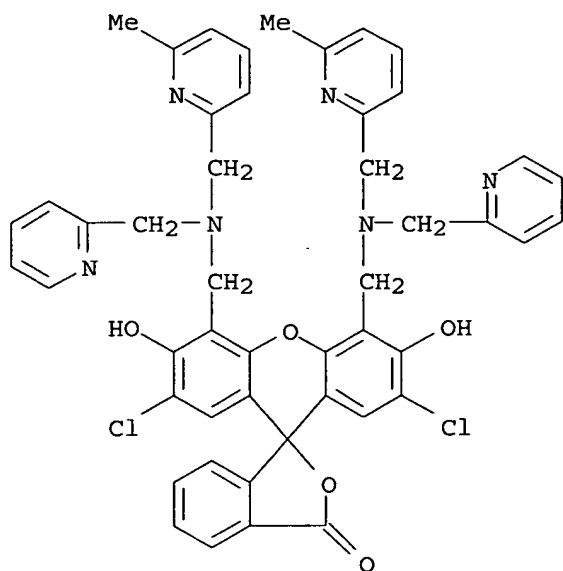
IT **877375-13-8P 877375-14-9P**

RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

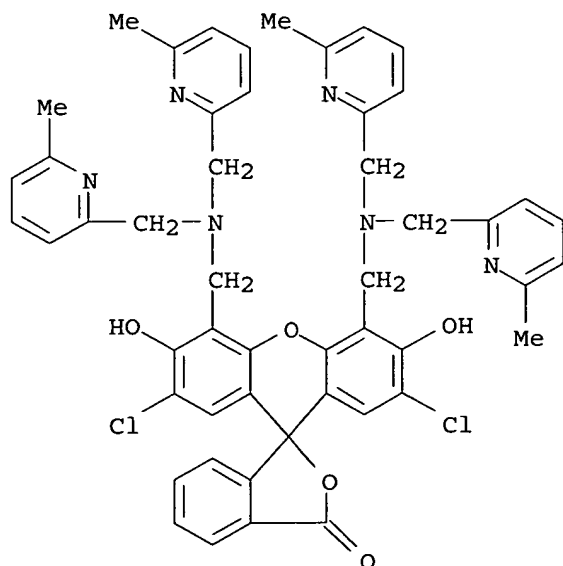
(preparation, chemical photophys., and Zn-responsive **fluorescence** properties of methylated derivs. of zinpyr ZP 1 zinc sensor)

RN 877375-13-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



RN 877375-14-9 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER (3) OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1192468 CAPLUS

DOCUMENT NUMBER: 144:83829

TITLE: QZ1 and QZ2: Rapid, Reversible Quinoline-Derivatized Fluoresceins for Sensing Biological Zn(II)

AUTHOR(S) : Nolan, Elizabeth M.; Jaworski, Jacek; Okamoto,  
Kenichi; Hayashi, Yasunori; Sheng, Morgan; Lippard,  
Stephen J.



CORPORATE SOURCE: Departments of Chemistry and Brain and Cognitive Sciences, Picower Institute for Learning and Memory, RIKEN-MIT Neuroscience Research Center, Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (2005), 127(48), 16812-16823  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB QZ1, 2-[2-chloro-6-hydroxy-3-oxo-5-(quinolin-8-ylaminomethyl)-3H-xanthen-9-yl]benzoic acid, and QZ2, 2-[6-hydroxy-3-oxo-4,5-bis-(quinolin-8-ylaminomethyl)-3H-xanthen-9-yl]benzoic acid, two **fluorescein**-based dyes derivatized with 8-aminoquinoline, have been prepared and their photophys., thermodyn., and zinc-binding kinetic properties determined. Because of their low background **fluorescence** and highly emissive Zn(II) complexes, QZ1 and QZ2 have a large dynamic range, with .apprx.42- and .apprx.150-fold **fluorescence** enhancements upon Zn(II) coordination, resp. These dyes have micromolar K<sub>d</sub> values for Zn(II) and are selective for Zn(II) over biol. relevant concns. of the alkali and alkaline earth metals. The Zn(II) complexes also **fluoresce** brightly in the presence of excess Mn(II), Fe(II), Co(II), Cd(II), and Hg(II), offering improved specificity for Zn(II) over di(2-picolyl)amine-based Zn(II) sensors. Stopped-flow kinetic investigations indicate that QZ1 and QZ2 bind Zn(II) with kon values of (3-4) + 10<sup>6</sup> M<sup>-1</sup> s<sup>-1</sup>, compared to (6-8) + 10<sup>5</sup> M<sup>-1</sup> s<sup>-1</sup> for select ZP (Zinpyr) dyes, at 4.3°. Dissociation of Zn(II) from QZ1 and QZ2 occurs with koff values of 150 and 160 s<sup>-1</sup>, over 5 orders of magnitude larger than those for ZP probes, achieving reversibility on the biol. (millisecond) time scale. Laser scanning confocal and two-photon microscopy studies reveal that QZ2 is **cell**-permeable and Zn(II)-responsive in vivo. Because of its weaker affinity for Zn(II), QZ2 responds to higher concns. of **intracellular** Zn(II) than members of the ZP family, illustrating that binding affinity is an important parameter for Zn(II) detection in vivo.

CC 9-5 (Biochemical Methods)  
Section cross-reference(s): 28

ST QZ1 QZ2 quinoline derivatized **fluorescein** zinc sensor

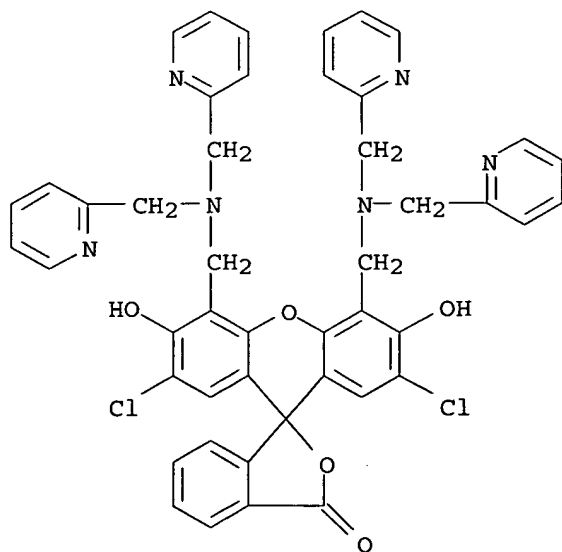
IT Affinity  
Complexation  
Confocal laser scanning microscopy  
Dissociation  
Dissociation constant  
Emissivity  
**Fluorescence**  
**Fluorescent** indicators  
**Fluorometry**  
HeLa cell  
Human  
UV and visible spectra  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))

IT pH  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II) in relation to)

IT Biosensors  
Imaging  
Optical sensors  
(**fluorescent**; QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))

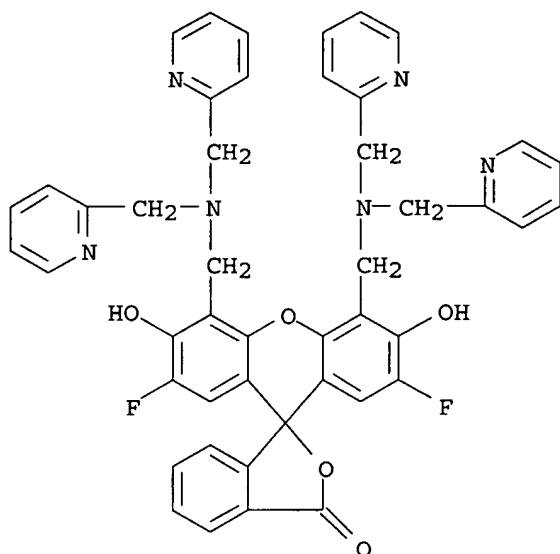
IT Biological transport

- (permeation; QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))
- IT **Fluorescence microscopy**  
(two-photon; QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))
- IT 7440-66-6, Zinc, analysis  
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))
- IT 872171-83-0P 872171-84-1P  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))
- IT 578-66-5, 8-Aminoquinoline 357615-03-3 389625-17-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II))
- IT 288574-78-7 502467-23-4 791072-81-6  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II) in relation to)
- IT 288574-78-7 791072-81-6  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(QZ1 and QZ2 as rapid, reversible quinoline-derivatized **fluoresceins** for sensing biol. Zn(II) in relation to)
- RN 288574-78-7 CAPLUS
- CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino)methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



- RN 791072-81-6 CAPLUS
- CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-

pyridinylmethyl)amino]methyl]-2',7'-difluoro-3',6'-dihydroxy- (9CI) (CA  
INDEX NAME)



REFERENCE COUNT: 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L79 ANSWER 4 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 20051122051 CAPLUS

DOCUMENT NUMBER: 144:56706

TITLE: Highly Effective **Fluorescent** and  
Colorimetric Sensors for **Pyrophosphate** over  
H<sub>2</sub>PO<sub>4</sub><sup>-</sup> in 100% Aqueous Solution

AUTHOR(S): Jang, Yun Jung; Jun, Eun Jin; Lee, Yoon Ju; Kim, Youn  
Sang; Kim, Jong Seung; Yoon, Juyoung

CORPORATE SOURCE: Department of Chemistry, Ewha Womans University,  
Seoul, 120-750, S. Korea

SOURCE: Journal of Organic Chemistry (2005), 70(23), 9603-9606  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Zinpyr-1·Zn<sup>2+</sup> acts as a **fluorescent** and colorimetric  
sensor for **pyrophosphate** at pH 7.4. Zinpyr-1·Cu<sup>2+</sup> and  
DIARB-1·Cu<sup>2+</sup> complexes act as selective **fluorescent**  
sensors for **pyrophosphate**. Also, the chemosensors  
Zinpyr-1·Zn<sup>2+</sup> and Zinpyr-1·Cu<sup>2+</sup> show highly selective and  
ratiometric **fluorescence** changes for **pyrophosphate**  
compared with H<sub>2</sub>PO<sub>4</sub><sup>-</sup>.

CC 61-3 (Water)

ST **pyrophosphate** detn aq soln **fluorescent** colorimetric  
sensor

IT Titration

(**fluorescence**; highly effective **fluorescent** and  
colorimetric sensors for **pyrophosphate** over dihydrogen  
**phosphate** in pure aqueous solution)

IT Colorimetric indicators

## Colorimetry

## Fluorescent indicators

## Fluorometry

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT Titration

(spectrophotometric; highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT 7732-18-5, Water, analysis

RL: AMX (Analytical matrix); ANST (Analytical study)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

IT 14000-31-8, **Pyrophosphate** 871233-74-8

RL: ANT (Analyte); ANST (Analytical study)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT 871233-70-4P 871233-71-5P 871233-72-6P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

IT 14066-20-7, **Phosphate** (H<sub>2</sub>PO<sub>4</sub><sup>-</sup>), analysis

RL: ARU (Analytical role, unclassified); ANST (Analytical study)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT 871233-73-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT 76-54-0, 2',7'-Dichlorofluorescein 6290-05-7, Diethyl iminodiacetate 288574-78-7, Zinpyr-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

## IT 871233-74-8

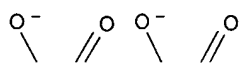
RL: ANT (Analyte); ANST (Analytical study)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

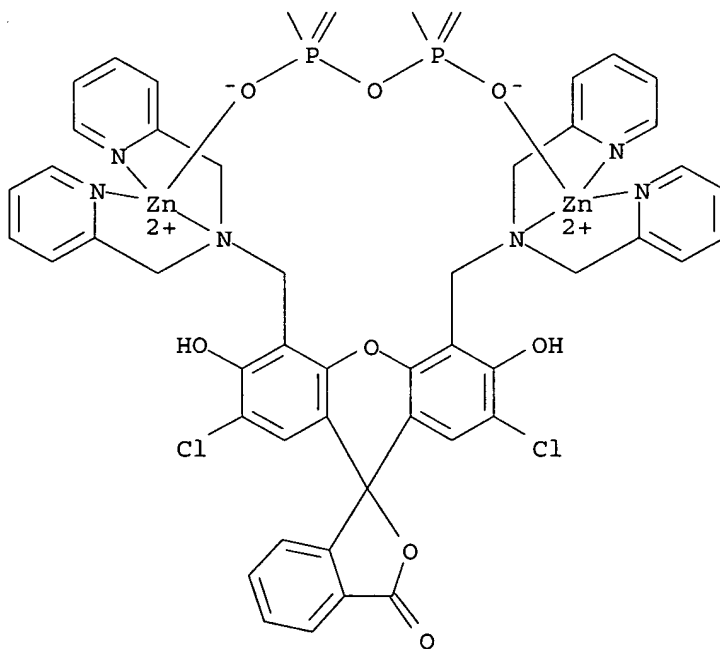
## RN 871233-74-8 CAPLUS

CN Zinc, [ $\mu$ -[4',5'-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-2',7'-dichloro-3',6'-dihydroxyspiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one]] [ $\mu$ -[diphosphato(4-)- $\kappa$ O: $\kappa$ O']]di-, monohydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



PAGE 3-A

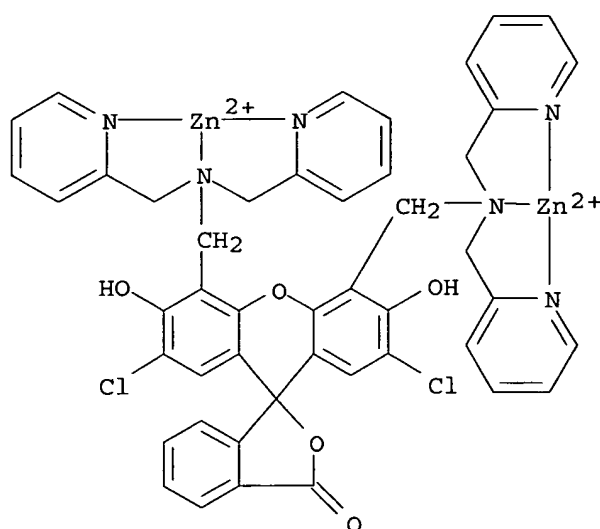
● H<sup>+</sup>

IT 871233-70-4P 871233-71-5P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (highly effective **fluorescent** and colorimetric sensors for  
**pyrophosphate** over dihydrogen **phosphate** in pure aqueous  
 solution)

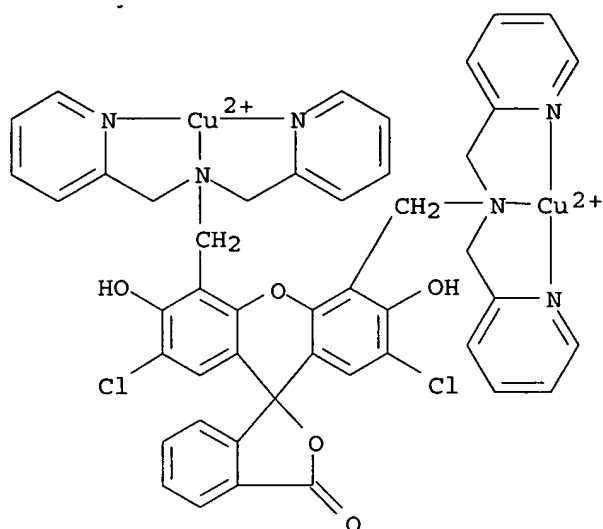
RN 871233-70-4 CAPLUS

CN Zinc(4+), [μ-[4',5'-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-2',7'-dichloro-3',6'-dihydroxyspiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one]]di- (9CI) (CA INDEX NAME)



RN 871233-71-5 CAPLUS

CN Copper(4+), [μ-[4',5'-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-2',7'-dichloro-3',6'-dihydroxyspiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one]]di- (9CI) (CA INDEX NAME)



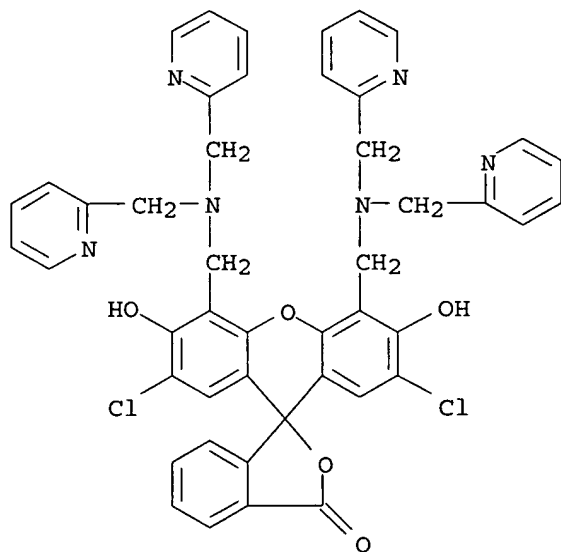
IT 288574-78-7, Zinpyr-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(highly effective **fluorescent** and colorimetric sensors for **pyrophosphate** over dihydrogen **phosphate** in pure aqueous solution)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 5 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2005-1094904 CAPLUS

DOCUMENT NUMBER: 144:63340  
 TITLE: Exogenous Nitrile Substrate Hydroxylation by a New Dicopper-Hydroperoxide Complex  
 AUTHOR(S): Li, Lei; Sarjeant, Amy A. Narducci; Vance, Michael A.; Zakharov, Lev. N.; Rheingold, Arnold L.; Solomon, Edward I.; Karlin, Kenneth D.  
 CORPORATE SOURCE: Department of Chemistry, The Johns Hopkins University, Baltimore, MD, 21218, USA  
 SOURCE: Journal of the American Chemical Society (2005), 127(44), 15360-15361  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A dicopper(I)/phenol-ligand complex,  $[\text{CuI}_2(\text{PD}'\text{OH})(\text{RCN})_2]^{2+}$  ( $\text{PD}'\text{OH}$  = 4-tert-butyl-2,6-bis[bis(2-pyridylethyl)amino]phenol) in RCN solvents reacts with  $\text{O}_2$  producing a  $\mu$ -1,1-hydroperoxo dicopper(II) species,  $[\text{CuII}_2(\text{PD}'\text{O}-)(\text{O}-\text{OH})]^{2+}$ . Subsequent thermal transformation results in nitrile hydroxylation and elimination of cyanide, as revealed by the isolation in comparable yields of (i) a cyanide-bridged tetranuclear cluster complex  $[\{\text{CuII}_2(\text{PD}'\text{O}-)(\text{CN})\}_2](\text{ClO}_4)_4$  and (ii) benzaldehyde (for  $\text{R} = \text{PhCH}_2$ ); 18O labeling confirms that the  $\text{PhC}(\text{O})\text{H}$  O atom is derived from  $\text{O}_2$ . X-ray crystal structures of  $[\text{CuI}_2(\text{PD}'\text{OH})(\text{PPh}_3)_2](\text{ClO}_4)_2$  and  $[\{\text{CuII}_2(\text{PD}'\text{O}-)(\text{CN})\}_2](\text{ClO}_4)_4$  were determined. The isotope effect of 18O2 during the nitrile oxygenation reaction was investigated.

CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 7, 67, 75

ST crystal structure copper phenol **phosphine** complex cyano phenolato cluster; copper hydroperoxo phenolato dinuclear complex prepn nitrile hydroxylation mechanism; monooxygenase copper enzyme mimic dicopper hydroperoxide complex

IT Crystal structure  
 Molecular structure  
 (of dinuclear copper(I) phenol **triphenylphosphine** complex and tetranuclear copper(II) phenolato cyanide-bridged cluster)

IT 548756-41-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of dinuclear copper(I) phenol nitrile/**triphenylphosphine** complexes, copper(II) hydroperoxide derivative, and tetranuclear copper(II) phenolato cyanide-bridged derivative)

IT 870248-68-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (formation and Raman spectra)

IT 870248-61-6P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (intermediate in reaction of dicopper(I) phenol nitrile complex with dioxygen and subsequent hydroxylation of exogenous nitriles as mimic of copper monooxygenases, and Raman spectra)

IT 870248-69-4P 870466-62-9P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)

IT 870248-67-2P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation and deuterium isotope effect in oxygenation of nitrile via dicopper(II) hydroperoxide intermediate as mimic of copper monooxygenases)



IT 870248-63-8P 870248-65-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 870248-60-5P

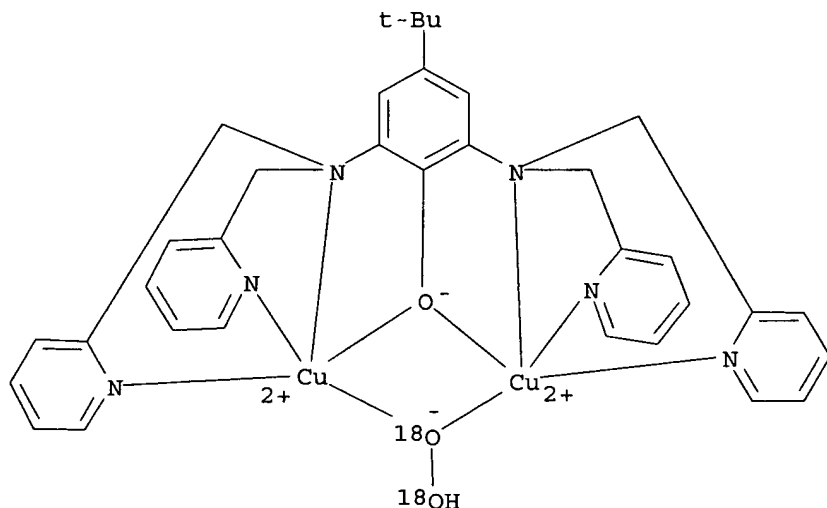
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(preparation, substitution with **triphenylphosphine**, and reactions with oxygen and nitriles via dicopper hydroperoxide intermediate as mimic of copper monooxygenases)

IT 870248-68-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(formation and Raman spectra)

RN 870248-68-3 CAPLUS

CN Copper(2+),  $[\mu\text{-}[2,6\text{-bis}[\text{bis}[(2\text{-pyridinyl-}\kappa\text{N})\text{methyl}]\text{amino-}\kappa\text{N}]\text{-4-(1,1-dimethylethyl)phenolato-}\kappa\text{O}:\kappa\text{O}]]\mu\text{-}(\text{hydroperoxy-1802-}\kappa\text{O}:\kappa\text{O})\text{di- (9CI) (CA INDEX NAME)}$

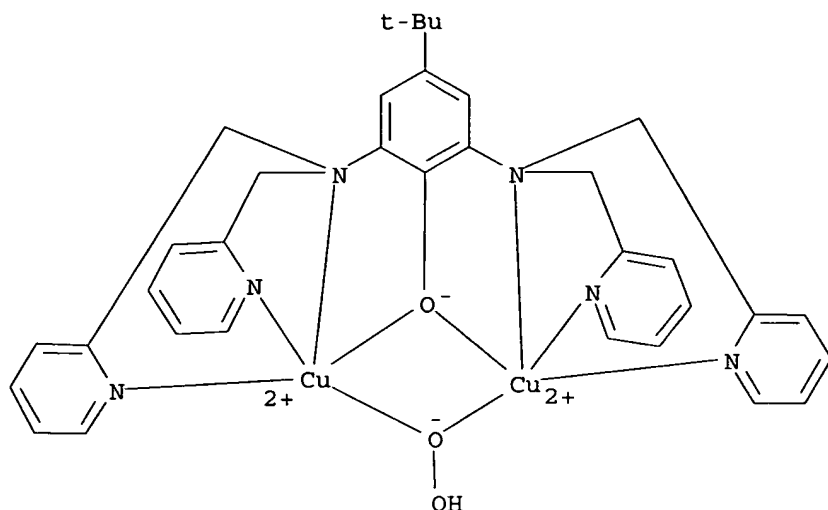


IT 870248-61-6P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(intermediate in reaction of dicopper(I) phenol nitrile complex with dioxygen and subsequent hydroxylation of exogenous nitriles as mimic of copper monooxygenases, and Raman spectra)

RN 870248-61-6 CAPLUS

CN Copper(2+),  $[\mu\text{-}[2,6\text{-bis}[\text{bis}[(2\text{-pyridinyl-}\kappa\text{N})\text{methyl}]\text{amino-}\kappa\text{N}]\text{-4-(1,1-dimethylethyl)phenolato-}\kappa\text{O}:\kappa\text{O}]]\mu\text{-}(\text{hydroperoxy-}\kappa\text{O}:\kappa\text{O})\text{di- (9CI) (CA INDEX NAME)}$



IT 870248-69-4P 870466-62-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

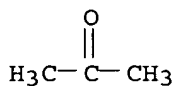
RN 870248-69-4 CAPLUS

CN Copper(2+), [μ-[2,6-bis[bis[(2-pyridinyl-κN)methyl]amino-κN]-4-(1,1-dimethylethyl)phenol]]bis(triphenylphosphine)di-,  
diperchlorate, compd. with 2-propanone (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 67-64-1

CMF C3 H6 O



CM 2

CRN 870248-65-0

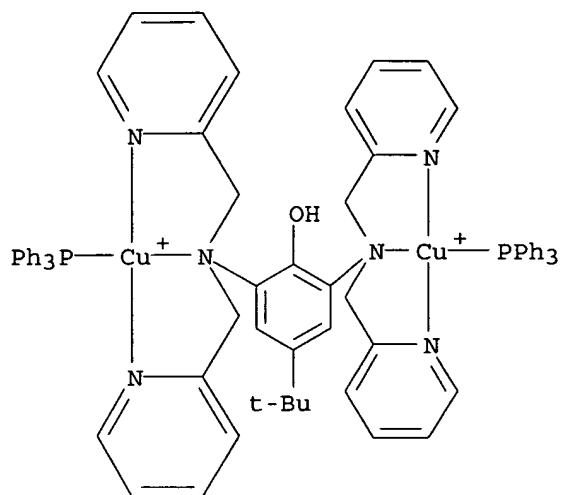
CMF C70 H66 Cu2 N6 O P2 . 2 Cl O4

CM 3

CRN 870248-64-9

CMF C70 H66 Cu2 N6 O P2

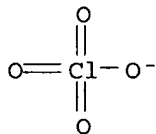
CCI CCS



CM 4

CRN 14797-73-0

CMF Cl O4

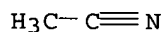


RN 870466-62-9 CAPLUS  
 CN Copper(4+), bis[μ-[2,6-bis[bis[(2-pyridinyl-κN)methyl]amino-κN]-4-(1,1-dimethylethyl)phenolato-κO:κO]]bis[μ-(cyano-κC:κN)]tetra-, cyclo, stereoisomer, tetraeperchlorate, compd. with acetonitrile (1:4) (9CI) (CA INDEX NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 870248-63-8

CMF C70 H70 Cu4 N14 O2 . 4 Cl O4

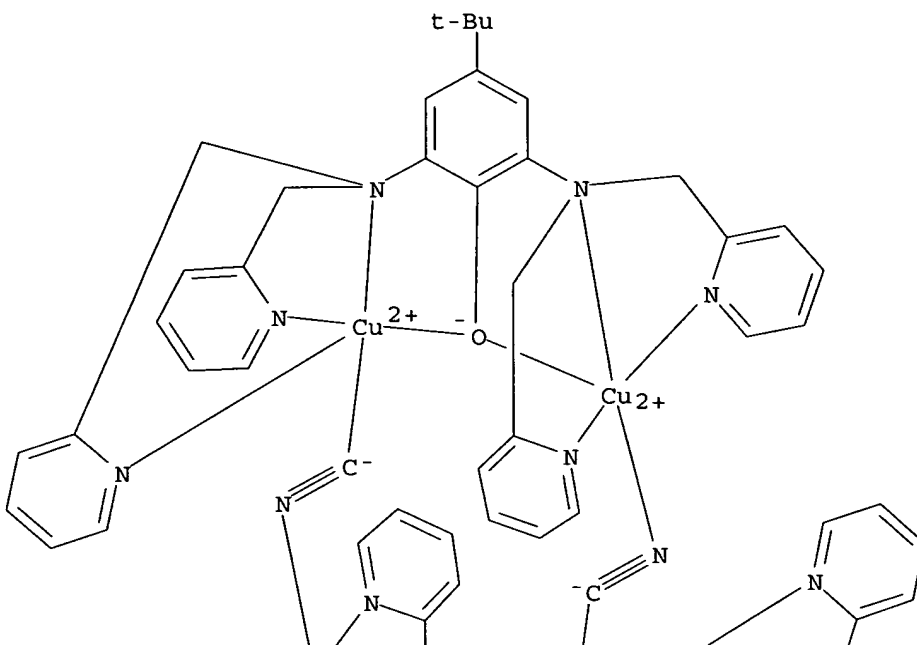
CM 3

CRN 870248-62-7

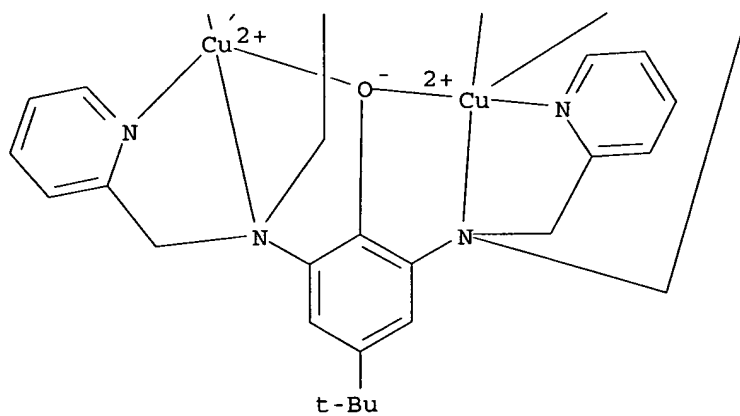
CMF C70 H70 Cu4 N14 O2

CCI CCS

PAGE 1-A



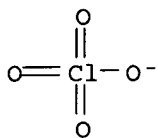
PAGE 2-A



CM 4

CRN 14797-73-0

CMF Cl O4



IT 870248-67-2P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation and deuterium isotope effect in oxygenation of nitrile via dicopper(II) hydroperoxide intermediate as mimic of copper monooxygenases)

RN 870248-67-2 CAPLUS

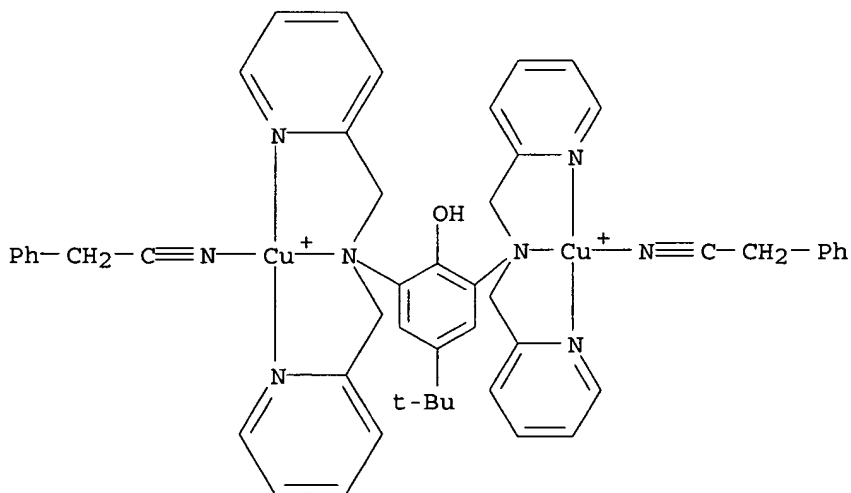
CN Copper(2+), bis(benzeneacetonitrile) [ $\mu$ -[2,6-bis[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]-4-(1,1-dimethylethyl)phenol]]di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 870248-66-1

CMF C50 H50 Cu2 N8 O

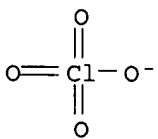
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 870248-63-8P 870248-65-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 870248-63-8 CAPLUS

CN Copper(4+), bis[μ-[2,6-bis[bis[(2-pyridinyl-κN)methyl]amino-κN]-4-(1,1-dimethylethyl)phenolato-κO:κO]]bis[μ-(cyano-κC:κN)]tetra-, cyclo, stereoisomer, tetra-perchlorate (9CI) (CA INDEX NAME)

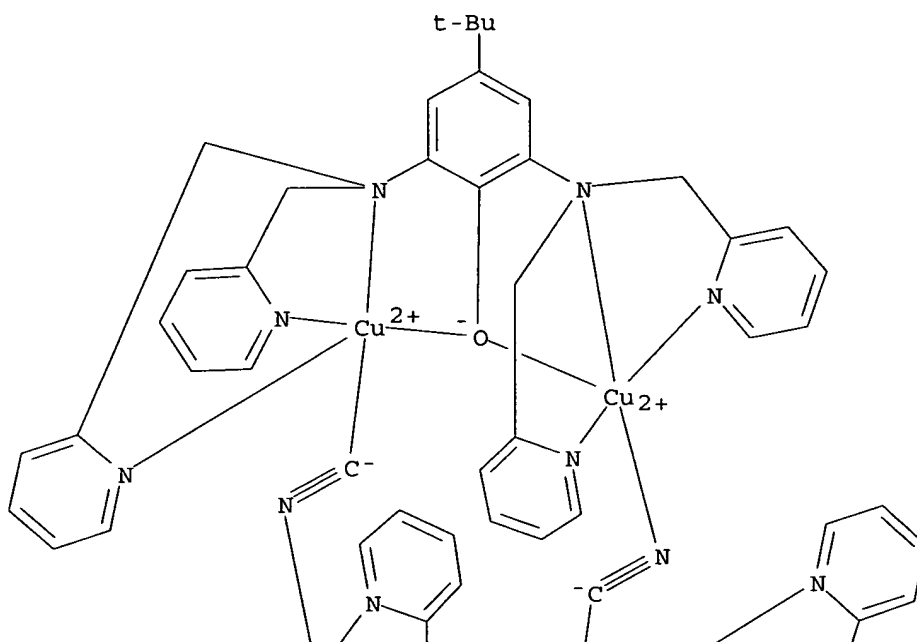
CM 1

CRN 870248-62-7

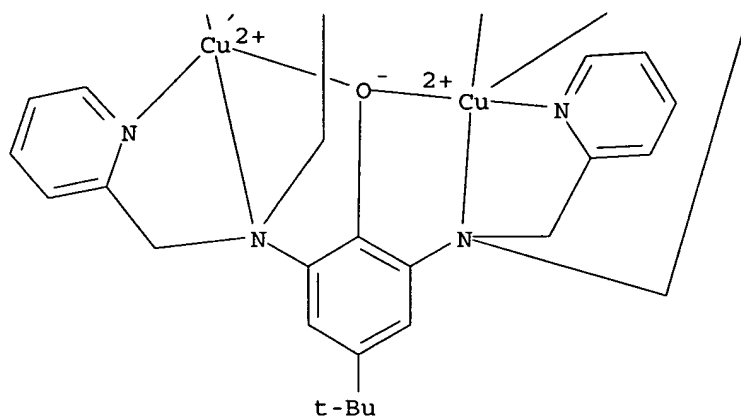
CMF C70 H70 Cu4 N14 O2

CCI CCS

PAGE 1-A



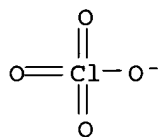
PAGE 2-A



CM 2

CRN 14797-73-0

CMF Cl O4



RN 870248-65-0 CAPLUS

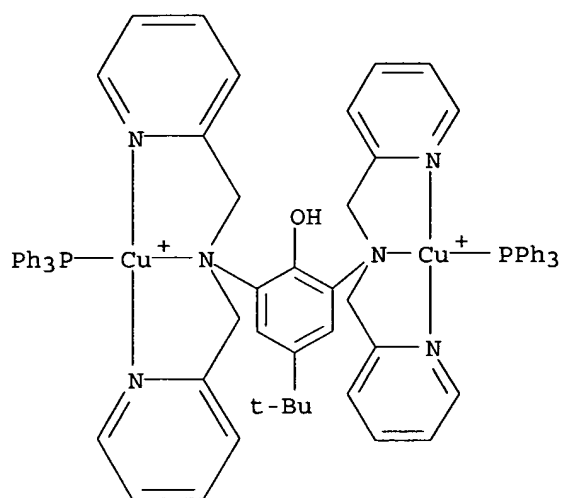
CN Copper(2+), [ $\mu$ -[2,6-bis[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]-4-(1,1-dimethylethyl)phenol]]bis(triphenylphosphine)di-,  
diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 870248-64-9

CMF C70 H66 Cu2 N6 O P2

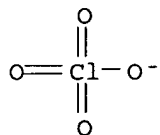
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 870248-60-5P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation, substitution with triphenylphosphine, and reactions with oxygen and nitriles via dicopper hydroperoxide intermediate as mimic of copper monooxygenases)

RN 870248-60-5 CAPLUS

CN Copper(2+), bis(acetonitrile) [ $\mu$ -[2,6-bis[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]-4-(1,1-dimethylethyl)phenol]]di-, diperchlorate (9CI) (CA INDEX NAME)

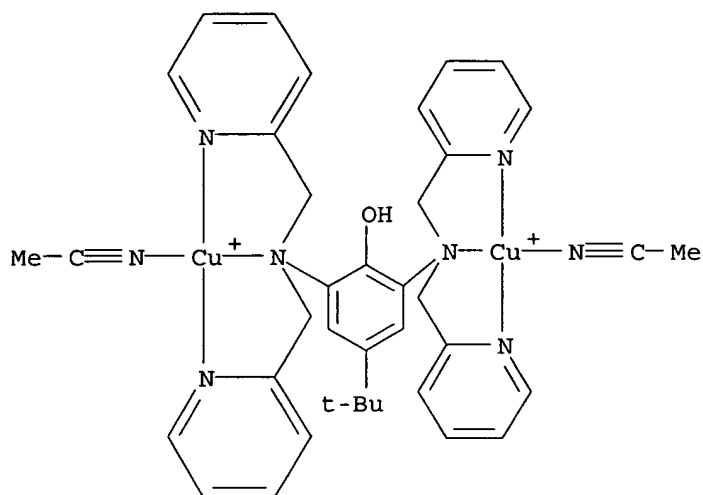
CM 1

CRN 870248-59-2

CMF C38 H42 Cu2 N8 O

CCI CCS

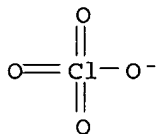




CM 2

CRN 14797-73-0

CMF Cl O4



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 6 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1065660 CAPLUS

DOCUMENT NUMBER: 144:15964

TITLE: Catalytic Transesterification of Dialkyl  
Phosphates by a Bioinspired Dicopper(II)  
Macrocyclic Complex

AUTHOR(S): Jagoda, Malgorzata; Warzeska, Sabine; Pritzkow, Hans;  
Wadepohl, Hubert; Imhof, Petra; Smith, Jeremy C.;  
Kraemer, Roland

CORPORATE SOURCE: Anorganisch-Chemisches Institut, The Universitaet  
Heidelberg, Heidelberg, 69120, Germany

SOURCE: Journal of the American Chemical Society (2005),  
127(43), 15061-15070

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB For a number of **phosphoryl** transfer enzymes, including the  
exonuclease subunit of DNA polymerase I, a mechanism involving two-metal  
ions and double Lewis-acid activation of the substrate, combined with  
leaving group stabilization, is proposed. Inspired by the active site  
structure of this enzyme, the authors have designed as a synthetic

**phosphoryl** transfer catalyst the dicopper(II) macrocyclic complex LCu<sub>2</sub>. Crystal structures of [(L)Cu<sub>2</sub>(μ-NO<sub>3</sub>)(NO<sub>3</sub>)](NO<sub>3</sub>)<sub>2</sub> (1), [(L)Cu<sub>2</sub>(μ-CO<sub>3</sub>)(CH<sub>3</sub>OH)](BF<sub>4</sub>)<sub>2</sub> (2), and [(L)Cu<sub>2</sub>(μ-O<sub>2</sub>P(OCH<sub>3</sub>)<sub>2</sub>)(NO<sub>3</sub>)](NO<sub>3</sub>)<sub>2</sub> (3) illustrate various possibilities for the interaction of oxoanions with the dicopper(II) site. 1 Efficiently promotes the transesterification of di-Me **phosphate** (DMP) in CD<sub>3</sub>OD, k<sub>cat</sub> = 2 × 10<sup>-4</sup> s<sup>-1</sup> at 55°. 1 Is the only available catalyst for the smooth transesterification of highly inert simple dialkyl **phosphates**. From photometric titrns. and the pH dependence of reactivity, [(L)Cu<sub>2</sub>(DMP)(OCH<sub>3</sub>)]<sup>2+</sup> is the reactive species. Steric bulk at the -OR substituents of **phosphodiester** substrates O<sub>2</sub>P(OR)<sub>2</sub> drastically reduces the reactivity of 1. This is explained with -OR leaving group stabilization by Cu coordination, an interaction which is sensitive to steric crowding at the α-C-atom of substituent R. A proposed reaction mechanism related to that of the exonuclease unit of DNA polymerase I is supported by DFT calcns. on reaction intermediates. [(L)Cu<sub>3</sub>(μ<sub>3</sub>-OH)(μ-CH<sub>3</sub>O)<sub>2</sub>(CH<sub>3</sub>CN)<sub>2</sub>](ClO<sub>4</sub>)<sub>3</sub> (4) incorporates a [Cu(OH)(OCH<sub>3</sub>)<sub>2</sub>(CH<sub>3</sub>CN)<sub>2</sub>]- complex anion, which might be considered as an analog of the [PO<sub>2</sub>(OCH<sub>3</sub>)<sub>2</sub>(OCD<sub>3</sub>)]<sup>2-</sup> transition state (or intermediate) of DMP transesterification catalyzed by LCu<sub>2</sub>.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 7, 29, 67, 75

IT Enzyme functional sites

(active; preparation, crystal structure and catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

IT Methanolysis kinetics

Steric hindrance

Transesterification

Transesterification catalysts

(preparation, crystal structure and catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

IT 9012-90-2, DNA polymerase

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

IT 2870-30-6, Sodium diethyl **phosphate** 4043-96-3, Sodium bis(p-nitrophenyl) **phosphate** 32586-82-6, Sodium dimethyl **phosphate** 32586-84-8 97174-13-5, Sodium dibenzyl **phosphate**

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

IT 869854-08-0P 869854-10-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

IT 363150-90-7P 869854-00-2P 869854-03-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of dinuclear copper(II) octaaza macrocycle complex)

IT 869853-95-2P

RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)

(preparation, crystal structure and catalytic transesterification of dialkyl

phosphates by dinuclear copper(II) octaaza macrocycle complex  
as model of phosphoryl transfer enzymes)

IT 363150-90-7P 869854-00-2P 869854-03-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of dinuclear copper(II) octaaza  
macrocycle complex)

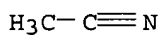
RN 363150-90-7 CAPLUS

CN Copper(3+), bis(acetonitrile)- $\mu_3$ -hydroxydi- $\mu$ -methoxy[ $\mu$ -  
(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.76,14.18,12.121,25.128,32.  
137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-  
dodecaene-3,16-diyne- $\kappa$ N1, $\kappa$ N19, $\kappa$ N34, $\kappa$ N35: $\kappa$ N6,  
 $\kappa$ N14, $\kappa$ N43, $\kappa$ N44)]tri-, stereoisomer, triperchlorate,  
compd. with acetonitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 363150-89-4

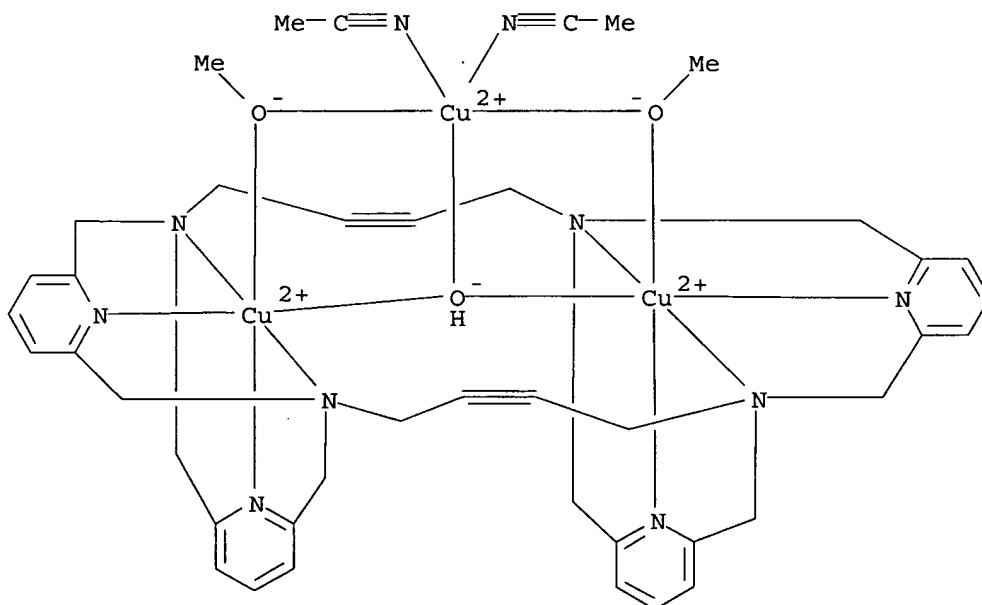
CMF C42 H49 Cu3 N10 O3 . 3 Cl O4

CM 3

CRN 363150-88-3

CMF C42 H49 Cu3 N10 O3

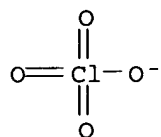
CCI CCS



CM 4

CRN 14797-73-0

CMF Cl O4



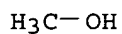
RN 869854-00-2 CAPLUS

CN Copper(2+), [ $\mu$ -[carbonato(2-)- $\kappa\text{O}:\kappa\text{O},\kappa\text{O}'$ ]](methanol)[.mu.-(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.76,14.18,12.121,25.128,32.137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-dodecaene-3,16-diyne- $\kappa\text{N1},\kappa\text{N19},\kappa\text{N34},\kappa\text{N35}:\kappa$ .N6, $\kappa\text{N14},\kappa\text{N43},\kappa\text{N44}$ )]di-, stereoisomer, bis[tetrafluoroborate(1-)], compd. with methanol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1

CMF C H4 O



CM 2

CRN 869853-99-6

CMF C38 H40 Cu2 N8 O4 . 2 B F4

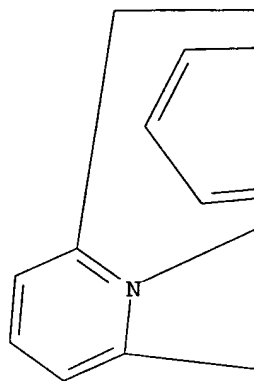
CM 3

CRN 869853-98-5

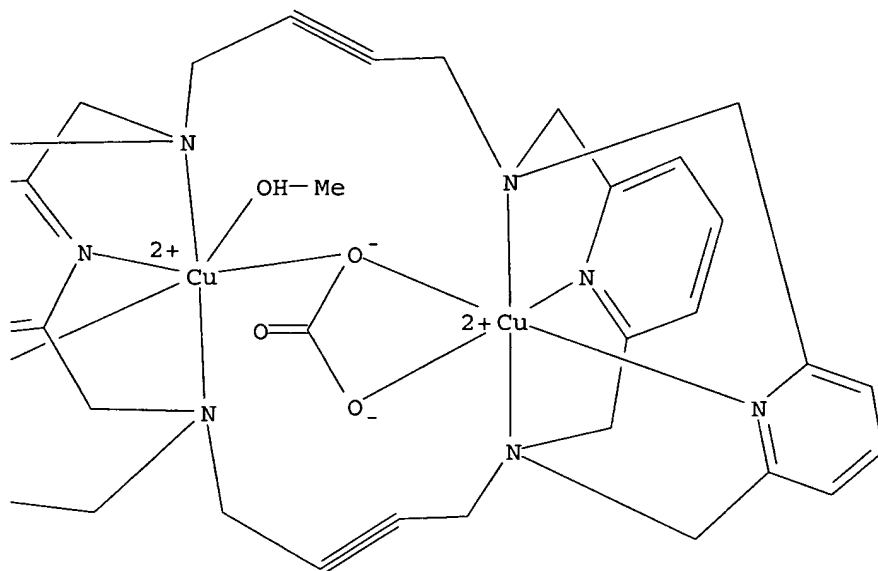
CMF C38 H40 Cu2 N8 O4

CCI CCS

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PAGE 1-B

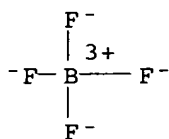


CM 4

CRN 14874-70-5

CMF B F4

CCI CCS

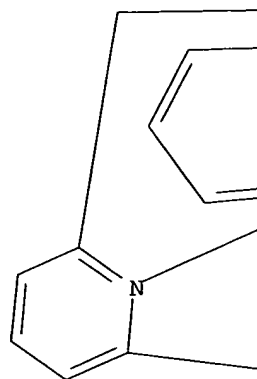


RN 869854-03-5 CAPLUS  
 CN Copper(2+), [ $\mu$ -(dimethyl phosphato- $\kappa\text{O}''':\kappa\text{O}''')$ ](nitrato- $\kappa\text{O}$ ) [ $\mu$ -(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.7.6,14.18,12.121,25.128,32.137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-dodecaene-3,16-diyne- $\kappa\text{N}1,\kappa\text{N}19,\kappa\text{N}34,\kappa$ .kappa.N35: $\kappa\text{N}6,\kappa\text{N}14,\kappa\text{N}43,\kappa\text{N}44$ )]di-, stereoisomer, dinitrate, compd. with methanol (1:1), monohydrate (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 67-56-1  
 CMF C H4 O

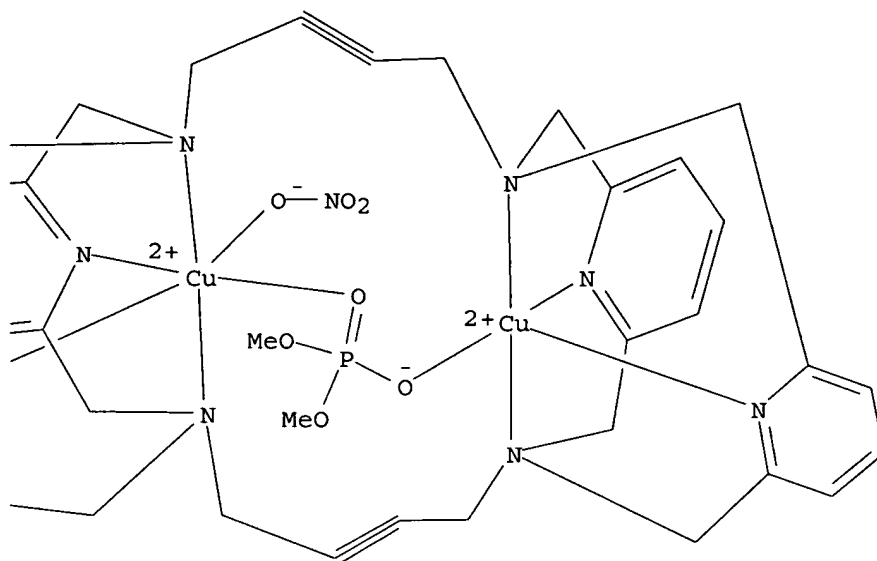
H<sub>3</sub>C-OH

CM 2  
 CRN 869854-02-4  
 CMF C38 H42 Cu2 N9 O7 P . 2 N O3  
 CM 3  
 CRN 869854-01-3  
 CMF C38 H42 Cu2 N9 O7 P  
 CCI CCS

PAGE 1-A



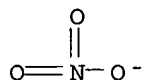
PAGE 1-B



CM 4

CRN 14797-55-8

CMF N O3



IT 869853-95-2P

RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)

(preparation, crystal structure and catalytic transesterification of dialkyl **phosphates** by dinuclear copper(II) octaaza macrocycle complex as model of **phosphoryl** transfer enzymes)

RN 869853-95-2 CAPLUS

CN Copper(2+), [ $\mu$ -(nitrato- $\kappa$ O: $\kappa$ O', $\kappa$ O')](nitrato- $\kappa$ O) [ $\mu$ -(1,6,14,19,34,35,43,44-octaazaheptacyclo[17.7.7.7.6,14.18,12.121,25.128,32.137,41]tetratetraconta-8,10,12(43),21,23,25(35),28,30,32(34),37,39,41(44)-dodecaene-3,16-diyne- $\kappa$ N1, $\kappa$ N19, $\kappa$ N34,.kappa.N35: $\kappa$ N6, $\kappa$ N14, $\kappa$ N43, $\kappa$ N44)]di-, stereoisomer, dinitrate, compd. with methanol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1

CMF C H4 O

H<sub>3</sub>C—OH

CM 2

CRN 869853-94-1

CMF C36 H36 Cu2 N10 O6 . 2 N O3

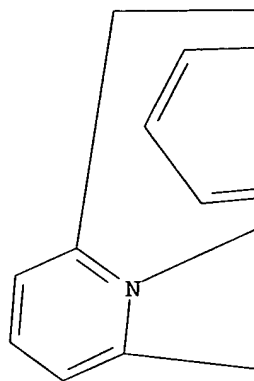
CM 3

CRN 869853-93-0

CMF C36 H36 Cu2 N10 O6

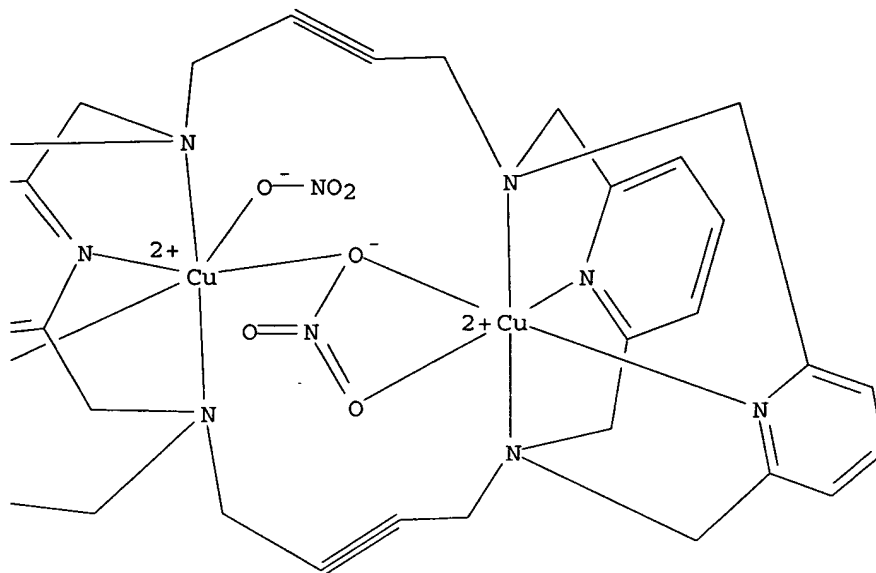
CCI CCS

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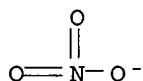
PAGE 1-B



CM 4

CRN 14797-55-8

CMF N O3



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 7 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:574969 CAPLUS

DOCUMENT NUMBER: 143:240739

TITLE: Dinuclear Mn(II), Ni(II), and Zn(II) complexes bridged by bis(p-nitrophenyl) **phosphate** ion: Relevance to bimetallic **phosphodiesterase**

AUTHOR(S): Shiraishi, Hitomi; Jikido, Reiko; Matsufuji, Kanako; Nakanishi, Tatsuki; Shiga, Takuya; Ohba, Masaaki; Sakai, Ken; Kitagawa, Hiroshi; Okawa, Hisashi

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Kyushu University, Fukuoka, 812-8581, Japan

SOURCE: Bulletin of the Chemical Society of Japan (2005), 78(6), 1072-1076

CODEN: BCSJA8; ISSN: 0009-2673

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:240739

AB 2,6-Bis[N,N-di(2-pyridylmethyl)aminomethyl]-4-methylphenol (Hbpm) has afforded dinuclear Mn(II), Ni(II), and Zn(II) complexes with two

bis(p-nitrophenyl) **phosphate** (BNP-) ions, [M2(bpmp)(bnp)2]ClO4  
(M = Mn (1), Ni (2), Zn (3)). The structure of 1·2MeCN was determined  
by the single crystal x-ray method. It has a dinuclear core structure  
bridged by the phenolic O atom of bpmp- and two BNP- ions. Each metal  
center has a pseudo octahedral geometry with an average Mn-to-donor bond  
distance of 2.207 Å. Physicochem. properties of 1-3 were studied and  
their relevance to biol. **phosphodiesterase** is discussed.

CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 75, 77

ST transition metal pyridylmethylaminomethylphenol  
**nitrophenylphosphate** prepn magnetic susceptibility; crystal  
structure manganese pyridylmethylaminomethylphenol  
**nitrophenylphosphate** bridged dinuclear

IT Antiferromagnetic exchange  
Magnetic susceptibility  
(of manganese and nickel bis[N,N-di(pyridylmethyl)aminomethyl]methylphe  
nol and bis(p-nitrophenyl)**phosphate** bridged dinuclear  
complexes)

IT Crystal structure  
Molecular structure  
(of manganese bis[N,N-di(pyridylmethyl)aminomethyl]methylphenol and  
bis(p-nitrophenyl)**phosphate** bridged dinuclear complex)

IT 4043-96-3, Sodium bis(p-nitrophenyl) **phosphate**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(complexation with transition metal ions)

IT 862686-81-5P **862686-83-7P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and magnetic properties)

IT 9025-82-5, **Phosphodiesterase**  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of dinuclear Mn(II), Ni(II), and Zn(II) bis[N,N-  
di(pyridylmethyl)aminomethyl]methylphenol and bis(p-nitrophenyl)  
**phosphate** bridged dinuclear complexes in relation to)

IT **862686-83-7P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and magnetic properties)

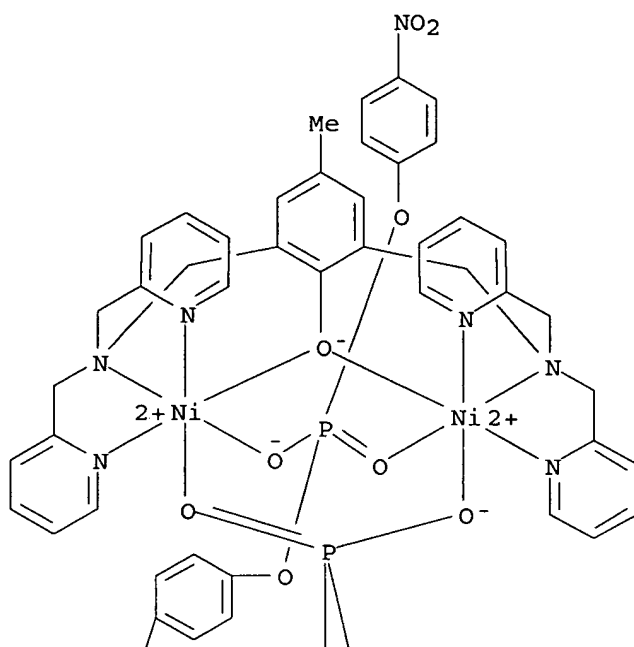
RN 862686-83-7 CAPLUS

CN Nickel(1+), [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-  
κN)methyl]-4-methylphenolato-κO:κO]]bis[μ-[bis(4-  
nitrophenyl) phosphato-κO':κO'']]di-, perchlorate (9CI) (CA  
INDEX NAME)

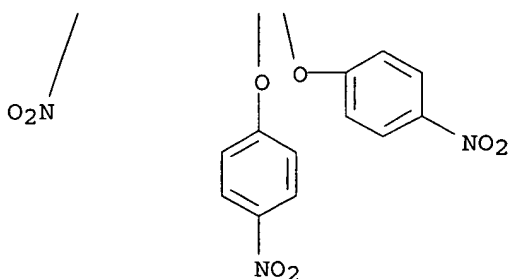
CM 1

CRN 862686-82-6  
CMF C57 H49 N10 Ni2 O17 P2  
CCI CCS

PAGE 1-A



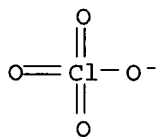
PAGE 2-A



CM 2

CRN 14797-73-0

CMF Cl O4



REFERENCE COUNT:

41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER '8 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:474990 CAPLUS

DOCUMENT NUMBER: 143:18749

TITLE: Novel dinuclear metal complex and  
**pyrophosphate** assay using the sameINVENTOR(S): Hong, Jong-In; Lee, Dong Hoon; Im, Ja Hyun; Son, Seung  
Uk; Chung, Young Keun

PATENT ASSIGNEE(S): S. Korea

SOURCE: U.S. Pat. Appl. Publ., 26 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

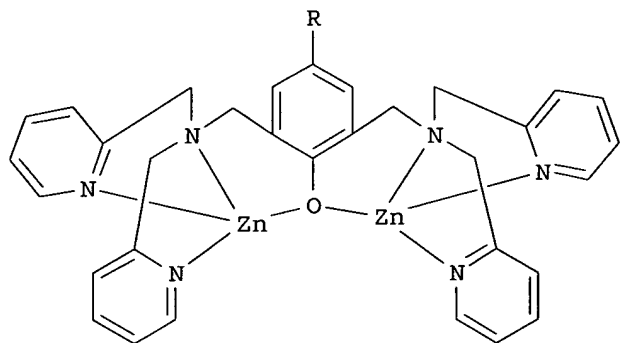
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE       |
|------------------------|------|----------|-----------------|------------|
| US 2005119497          | A1   | 20050602 | US 2004-855940  | 20040527   |
| PRIORITY APPLN. INFO.: |      |          | KR 2003-86782   | A 20031202 |
|                        |      |          | KR 2004-34773   | A 20040517 |

OTHER SOURCE(S): MARPAT 143:18749

GI



I

AB A novel coordination complex formed by dinuclear metal complexation is provided. The complex is a dinuclear metal complex of a compound, wherein the compound comprises a conjugation ring system substituted with: (a) an electron donating group selected from -OH, -SH and -NH<sub>2</sub>; (b) an indicating group selected from a chromogenic group, a **fluorescent** group and an electrochem. group; and (c) two binding auxiliary groups, in combination with the electron donating group each of which being coordinated with the metal to provide an anion bonding site, wherein as the complex binds to an anion, the coordination of the electron donating group with the metal is weakened and electron donation of the electron donating group to the conjugation ring system is reinforced, such that the reinforced electron donation by the electron donating group is transferred through the conjugation ring system to the indicating group to produce an indicating signal concomitant with the change of its electronic d. The coordination complex shows high sensitivity and high selectivity for **pyrophosphate** over other anions in an aqueous solvent over a wide pH range. Therefore, the complex is useful for **pyrophosphate** assay as a **pyrophosphate** sensor. Thus, zinc(II) complex I(NO<sub>3</sub>)<sub>3</sub> (R = 2-naphthyl) was prepared as a **fluorescent** sensor and I(NO<sub>3</sub>)<sub>3</sub> (R = C.tplbond.CFc, Fc = ferrocenyl) as an electrochem. sensor selective for

**pyrophosphate** assay. A sensor complex detected a small amount of **pyrophosphate** even in the presence of a large excess of ATP, thus the sensor could be used in bioanal. applications.

IC ICM C07F001-00

ICS D06L001-00

INCL 556034000

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 9, 27, 29, 73, 75, 79

ST **pyrophosphate** assay dinuclear transition metal pyridylmethylaminophenolate chelate sensor; zinc pyridylmethylaminophenolate dinuclear chelate sensor **pyrophosphate**; **diphosphate** sensor dinuclear transition metal pyridylmethylaminophenolate chelate; crystal structure zinc pyridylmethylaminophenolate **diphosphate** dinuclear

IT Sensors

(dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate**)

IT Biosensors

(dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate** in presence of excess ATP)

IT Biochips

(dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates attached to biochips as sensors selective for **pyrophosphate**)

IT Optical sensors

(dinuclear zinc(II) bis[bis(pyridylmethyl)aminomethyl]phenolate chelates containing **fluorescent** groups as sensors selective for **pyrophosphate**)

IT Sensors

(electrochem.; dinuclear zinc(II) bis[bis(pyridylmethyl)aminomethyl]phenolate chelate containing pendant ferrocenyl groups as electrochem. sensor selective for **pyrophosphate**)

IT Redox reaction

(electrochem.; of dinuclear zinc(II) bis[bis(pyridylmethyl)aminomethyl]phenolate chelate containing pendant ferrocenyl groups as electrochem. sensor for **pyrophosphate**)

IT Crystal structure

Molecular structure

(of dinuclear zinc(II) bis[bis(pyridylmethyl)aminomethyl]phenolate **pyrophosphate** chelate)

IT Transition metal complexes

RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate**)

IT 852286-12-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (formation and association constant of)

IT 852404-93-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and coordination with **pyrophosphate**)

IT 852286-11-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

IT 852286-02-3P

RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT

(Reactant or reagent); USES (Uses)  
 (preparation as UV-visible sensor selective for **pyrophosphate**)

IT **852286-05-6P**  
 RL: ARG (Analytical reagent use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 (preparation as electrochem. sensor selective for **pyrophosphate**)

IT **852286-03-4P 852286-06-7P 852286-07-8P**  
**852286-08-9P 852286-09-0P 852286-10-3P**  
 RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation as **fluorescent** sensor selective for **pyrophosphate**)

IT 14000-31-8, **Pyrophosphate** tetraanion  
 RL: ANT (Analyte); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)  
 (preparation of dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate**)

IT 100-01-6, p-Nitroaniline, reactions 1271-47-2, Ethynylferrocene 1539-42-0, Bis(2-pyridylmethyl)amine 1829-37-4 32316-92-0, 2-Naphthylboronic acid 60041-69-2 206879-83-6 692729-58-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate**)

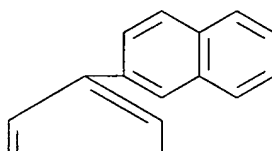
IT 444069-42-5P **569643-50-1P 792959-43-4P** 792959-45-6P  
 792959-47-8P 792959-49-0P **852285-95-1P** 852285-96-2P  
**852285-97-3P 852285-98-4P** 852285-99-5P 852286-00-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl]phenolate chelates as sensors selective for **pyrophosphate**)

IT **852286-12-5P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (formation and association constant of)

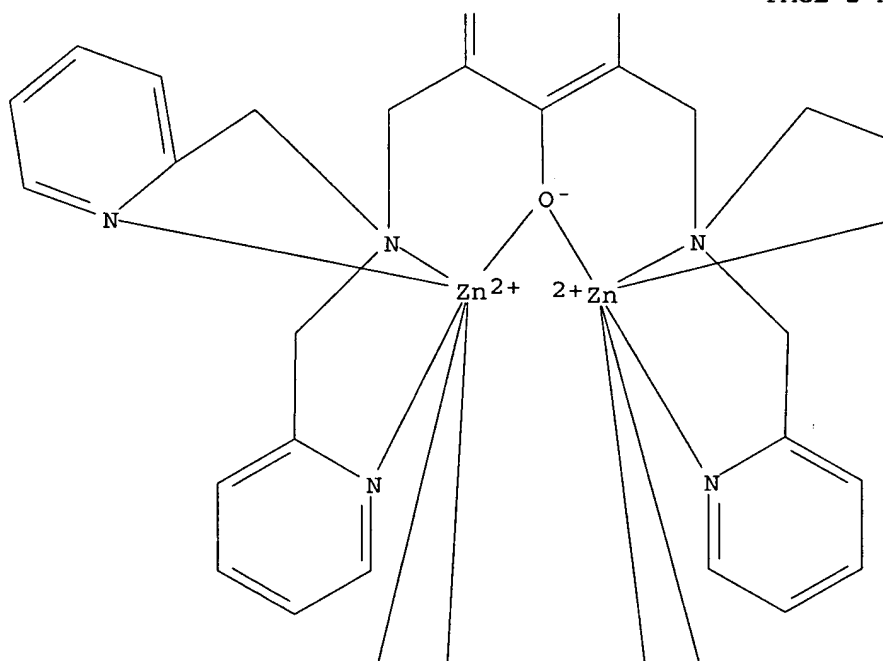
RN 852286-12-5 CAPLUS

CN Zincate(1-), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(2-naphthalenyl)phenolato- $\kappa$ O: $\kappa$ O]] [ $\mu$ -[diphosphato(4-)- $\kappa$ O, $\kappa$ O': $\kappa$ O', $\kappa$ O'']]di- (9CI) (CA INDEX NAME)

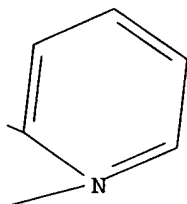
PAGE 1-A



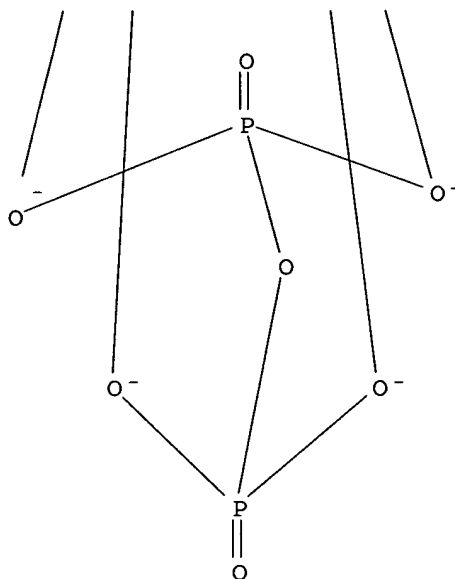
PAGE 2-A



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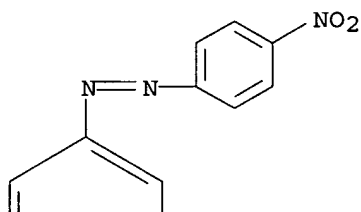
PAGE 3-A



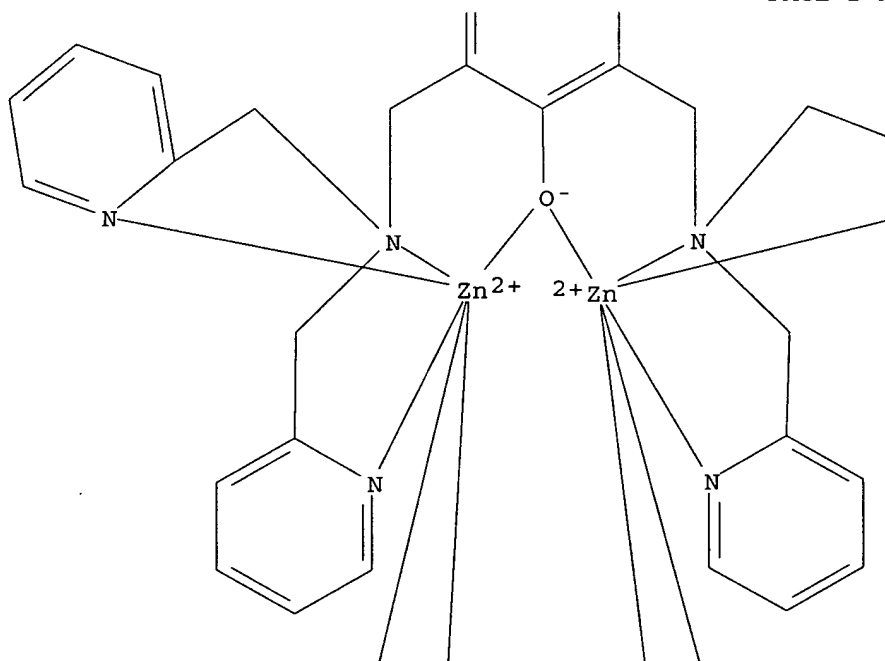
IT **852286-11-4P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 852286-11-4 CAPLUS  
 CN Zincate(1-), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato- $\kappa$ O: $\kappa$ O]] [ $\mu$ -[diphosphato(4-)- $\kappa$ O, $\kappa$ O': $\kappa$ O',.kappaappa.O''']]di-, potassium (9CI) (CA INDEX NAME)



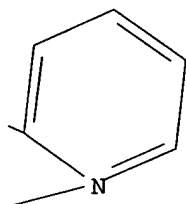
PAGE 1-A



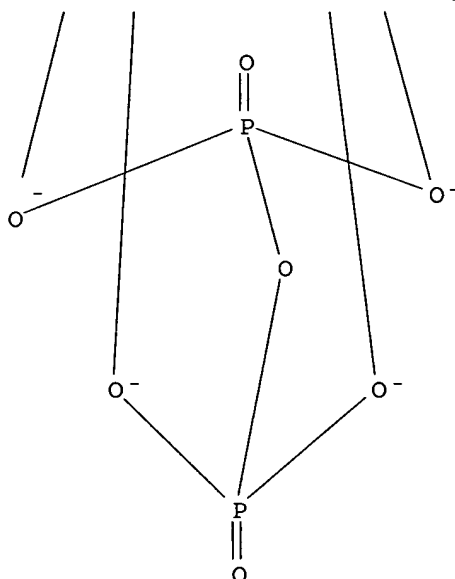
PAGE 2-A



PAGE 2-B



PAGE 3-A



PAGE 3-B

● K<sup>+</sup>

IT 852286-02-3P

RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation as UV-visible sensor selective for **pyrophosphate**)

RN 852286-02-3 CAPLUS

CN Zinc(3+), [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato-κO:κO]]di-, trinitrate (9CI) (CA INDEX NAME)

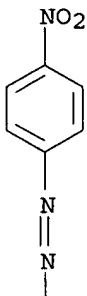
CM 1

CRN 852286-01-2

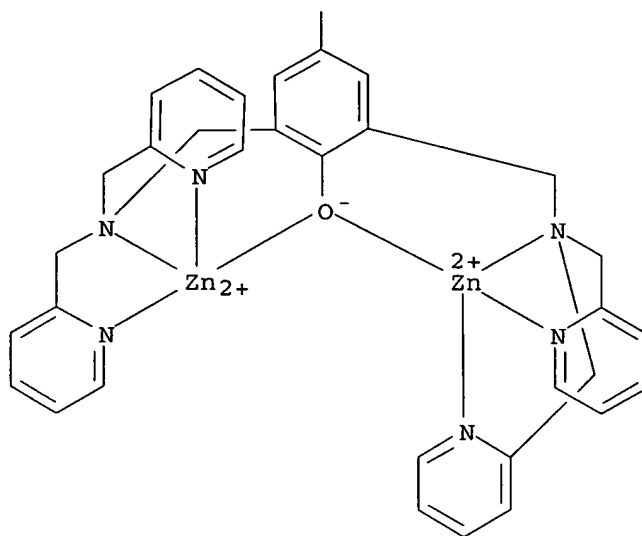
CMF C38 H34 N9 O3 Zn2

CCI CCS

PAGE 1-A



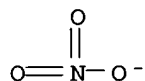
PAGE 2-A



CM 2

CRN 14797-55-8

CMF N O3



IT 852286-05-6P

RL: ARG (Analytical reagent use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
(preparation as electrochem. sensor selective for **pyrophosphate**)

RN 852286-05-6 CAPLUS

CN Zinc(3+), [ $\mu$ -[[3,5-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N]methyl]-4-(hydroxy- $\kappa$ O: $\kappa$ O)phenyl]ethynyl]ferrocenato]di-, trinitrate (9CI) (CA INDEX NAME)

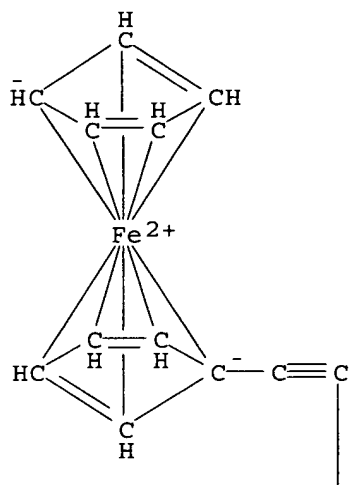
CM 1

CRN 852286-04-5

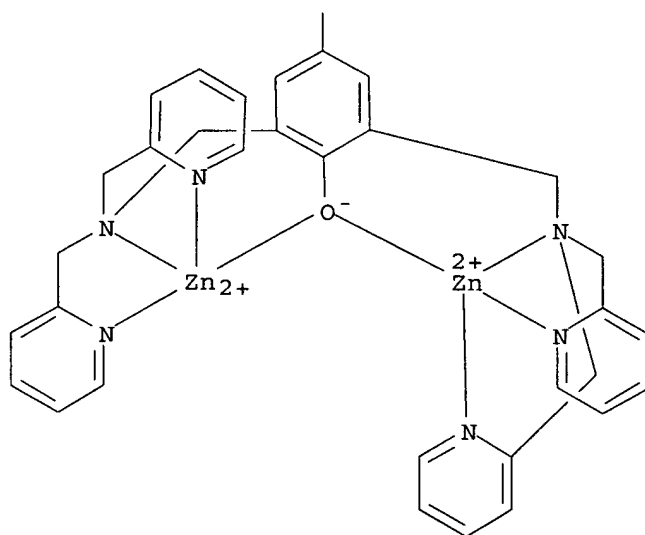
CMF C44 H39 Fe N6 O Zn2

CCI CCS

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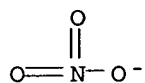
PAGE 2-A



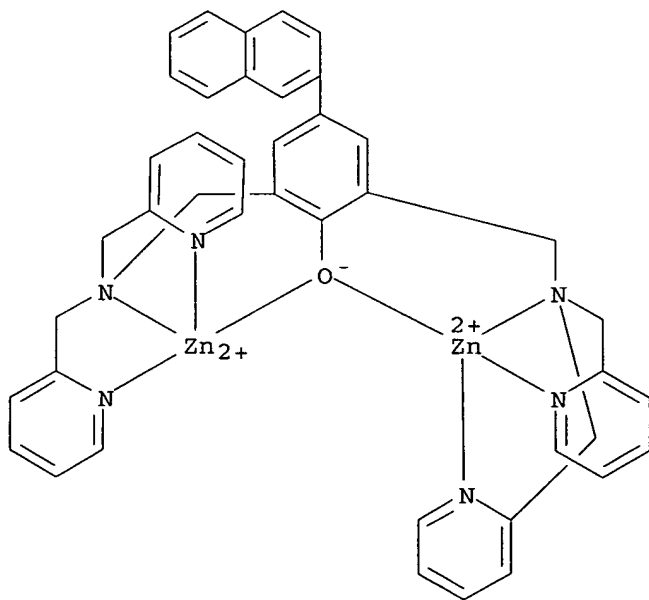
CM 2

CRN 14797-55-8

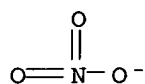
CMF N 03



IT 852286-03-4P 852286-06-7P 852286-07-8P  
 852286-08-9P 852286-09-0P 852286-10-3P  
 RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN  
 (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT  
 (Reactant or reagent); USES (Uses)  
 (preparation as **fluorescent** sensor selective for  
**pyrophosphate**)  
 RN 852286-03-4 CAPLUS  
 CN Zinc(3+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(2-naphthalenyl)phenolato- $\kappa$ O: $\kappa$ O]]di-,  
 trinitrate (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 793687-35-1  
 CMF C42 H37 N6 O Zn2  
 CCI CCS



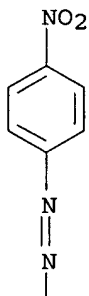
CM 2  
 CRN 14797-55-8  
 CMF N O3



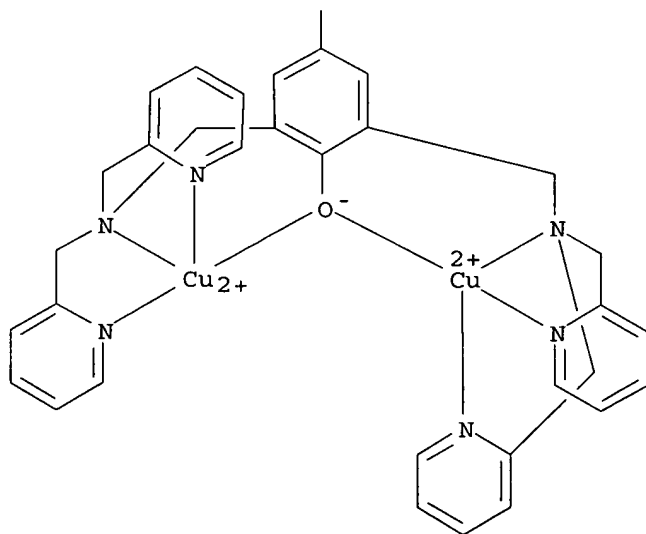
RN 852286-06-7 CAPLUS

CN Copper(3+),  $[\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato- $\kappa$ O: $\kappa$ O]]di-, stereoisomer (9CI) (CA INDEX NAME)

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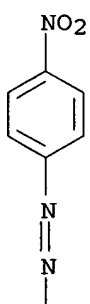


RN 852286-07-8 CAPLUS

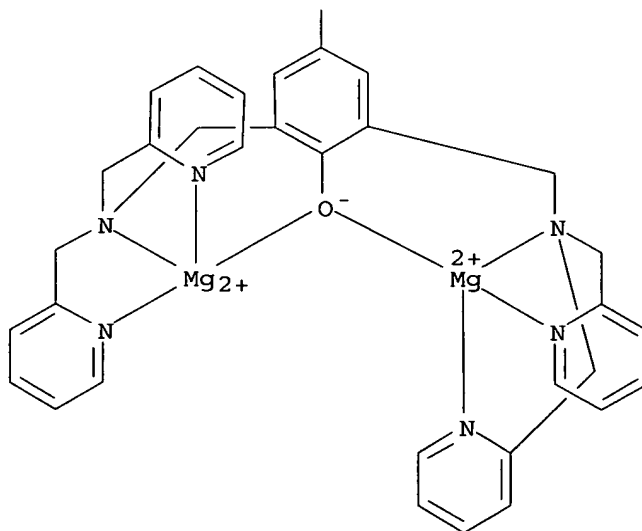
CN Magnesium(3+),  $[\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato-

$\kappa\text{O}:\kappa\text{O}] \text{di-}$  (9CI) (CA INDEX NAME)

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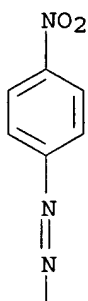
PAGE 2-A



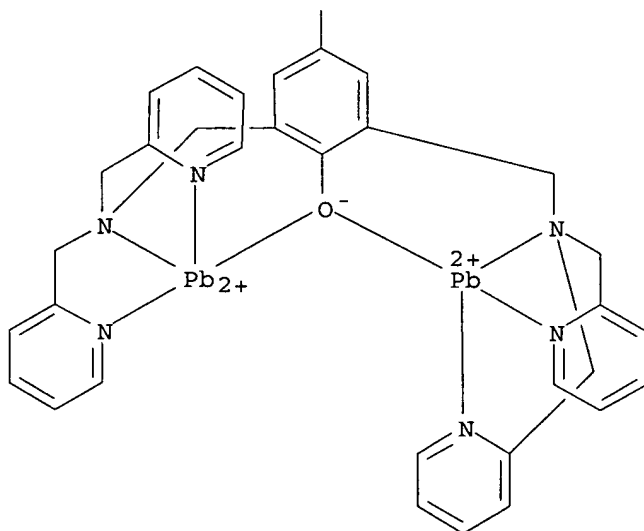
RN 852286-08-9 CAPLUS  
 CN Lead(3+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa\text{N}$ )methyl]amino- $\kappa\text{N}$ ]methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato- $\kappa\text{O}:\kappa\text{O}] \text{di-}$  (9CI) (CA INDEX NAME)



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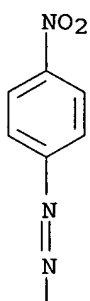


PAGE 2-A

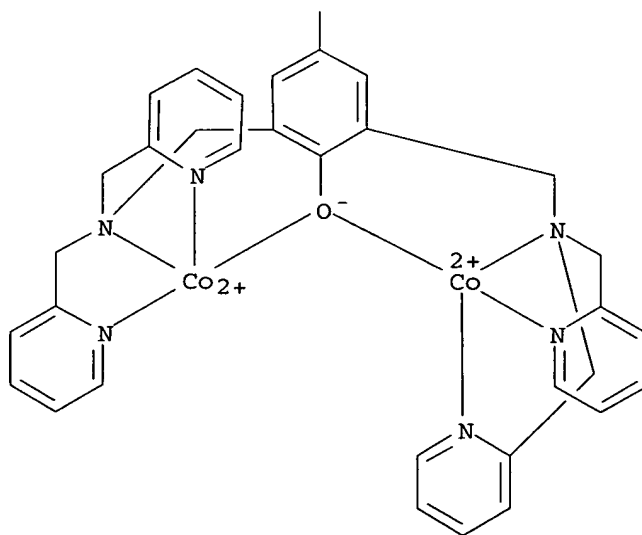


RN 852286-09-0 CAPLUS  
 CN Cobalt (3+), [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato-κO:κO]]di-, stereoisomer (9CI) (CA INDEX NAME)

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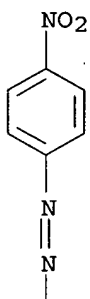


PAGE 2-A

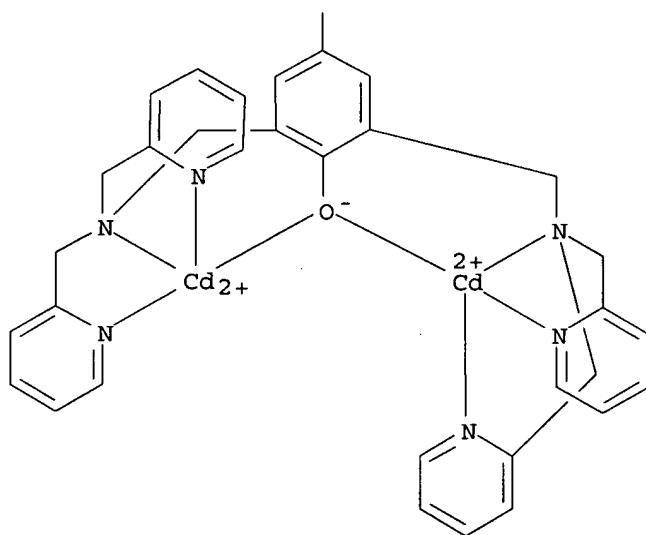


RN 852286-10-3 CAPLUS  
 CN Cadmium(3+), [μ-[2,6-bis[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-4-[(1E)-(4-nitrophenyl)azo]phenolato-κO:κO]]di- (9CI) (CA INDEX NAME)

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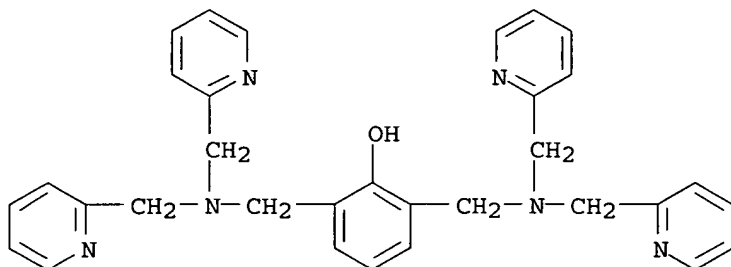
IT 569643-50-1P 792959-43-4P 852285-95-1P  
852285-97-3P 852285-98-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of dinuclear transition metal bis[bis(pyridylmethyl)aminomethyl  
phenolate chelates as sensors selective for **pyrophosphate**)

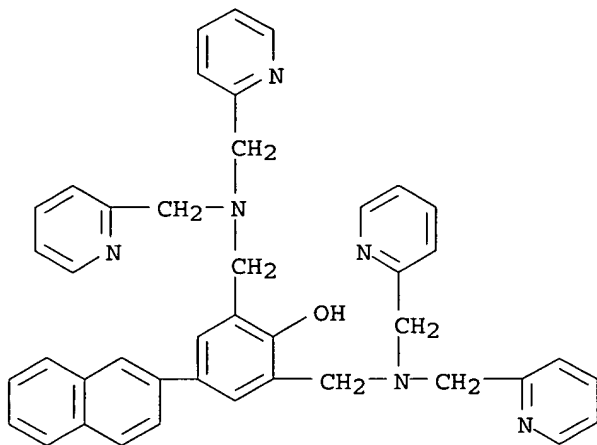
RN 569643-50-1 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl] - (9CI) (CA INDEX NAME)



RN 792959-43-4 CAPLUS

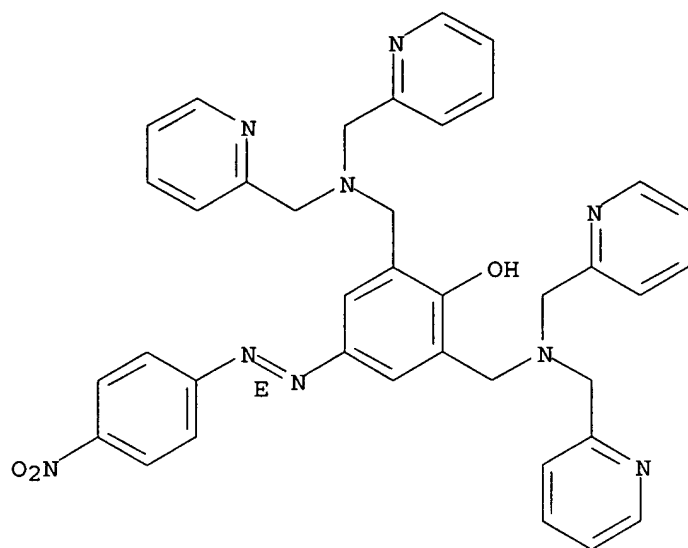
CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl] -4 - (2-naphthalenyl) - (9CI) (CA INDEX NAME)



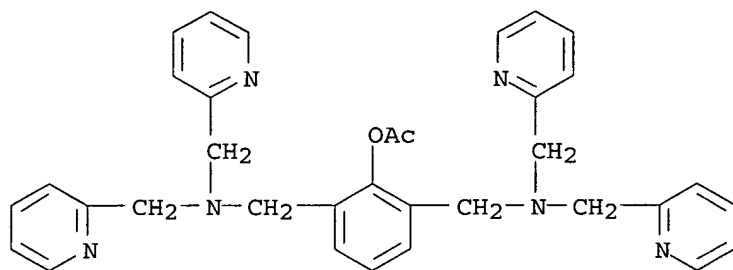
RN 852285-95-1 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl] -4 - [(1E) - (4-nitrophenyl)azo] - (9CI) (CA INDEX NAME)

Double bond geometry as shown.

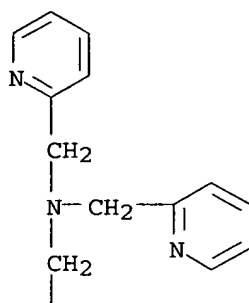


RN 852285-97-3 CAPLUS  
 CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-, acetate (ester)  
 (9CI) (CA INDEX NAME)

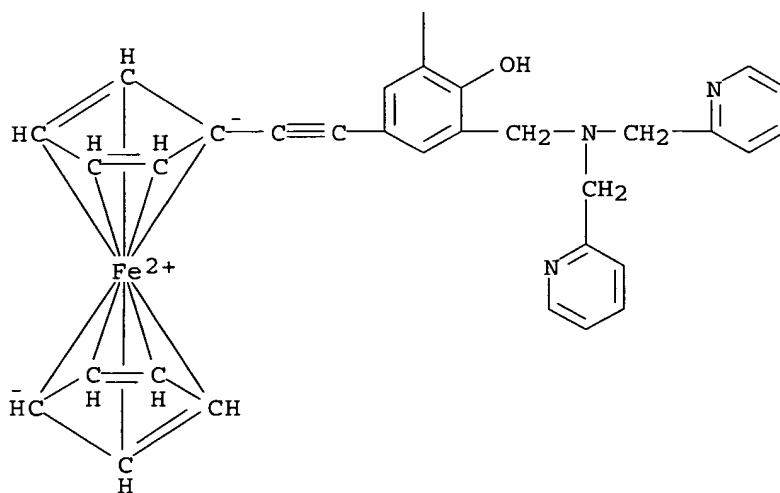


RN 852285-98-4 CAPLUS  
 CN Ferrocene, [[3,5-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-hydroxyphenyl]ethynyl]- (9CI) (CA INDEX NAME)

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L79 ANSWER 9 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:273930 CAPLUS

DOCUMENT NUMBER: 143:3598

TITLE: Esterase-activated two-fluorophore system  
for ratiometric sensing of biological zinc(II)AUTHOR(S): Woodroffe, Carolyn C.; Won, Annie C.; Lippard, Stephen  
J.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Inorganic Chemistry (2005), 44(9), 3112-3120  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB **Intracellular** ester hydrolysis by cytosolic esterases is a common strategy used to trap **fluorescent** sensors within the cell. We have prepared analogs of Zinpyr-1 (ZP1), an intensity-based **fluorescent** sensor for Zn<sup>2+</sup>, that are linked via an amido-ester or diester moiety to a calibrating **fluorophore**, coumarin 343. These compds., designated Coumazin-1 and -2, are nonpolar and are quenched by intramol. interactions between the two **fluorophores**. Esterase-catalyzed hydrolysis generates a Zn<sup>2+</sup>-sensitive ZP1-like **fluorophore** and a Zn<sup>2+</sup>-insensitive coumarin as a calibrating **fluorophore**. Upon excitation of the **fluorophores**, coumarin 343 emission relays information concerning sensor concentration whereas ZP1 emission indicates the relative concentration of Zn<sup>2+</sup>-bound sensor. This approach enables **intracellular** monitoring of total sensor concentration and provides a ratiometric system for sensing biol. zinc ion.

CC 9-14 (Biochemical Methods)

ST esterase **fluorophore** system ratiometric sensing biol zinc

IT **Fluorescent** substances  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT Imaging  
(**fluorescent**; esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT Sensors  
(**fluorometric**; esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT 7440-66-6, Zinc, analysis  
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT 144489-10-1  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT 55804-65-4P 615552-02-8P 616215-78-2P  
790660-95-6P 790661-00-6P 852299-72-0P  
852299-74-2P 852299-75-3P 852299-78-6P 852299-79-7P  
852299-80-0P 852299-81-1P 852299-82-2P  
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

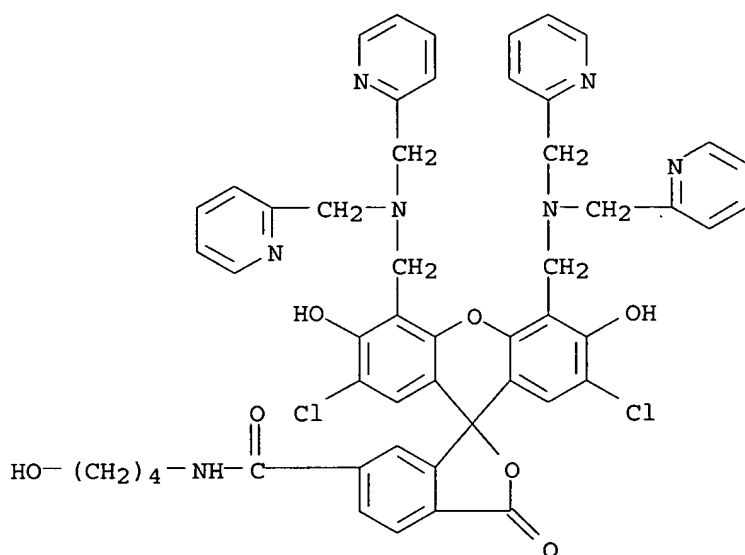
IT 9016-18-6, Esterase  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT 79-37-8, Oxalyl chloride 4541-14-4, 4-Benzoyloxy-1-butanol 25952-53-8,  
EDC 29227-68-7, Dipicolylamine 852299-76-4 852299-77-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(esterase-activated two-**fluorophore** system for ratiometric sensing of biol. zinc(II))

IT 615552-00-6P 790661-02-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (esterase-activated two-**fluorophore** system for ratiometric  
 sensing of biol. zinc(II))

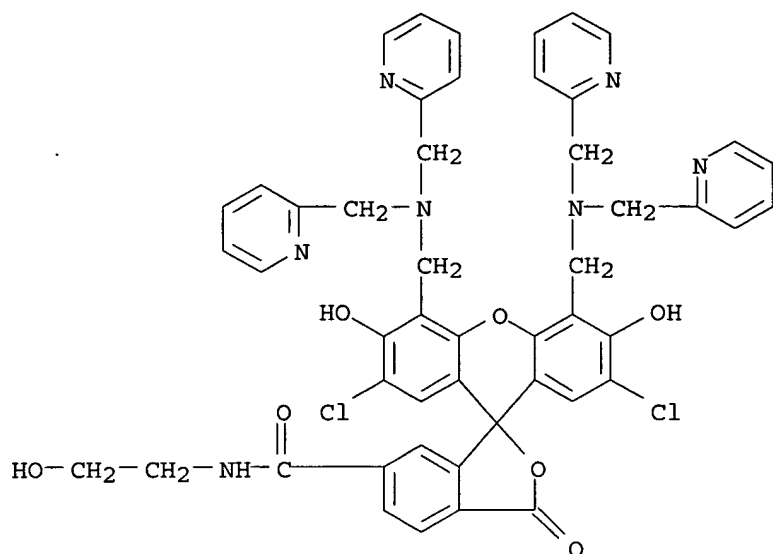
IT 615552-02-8P 616215-78-2P 790660-95-6P  
 852299-72-0P 852299-74-2P 852299-75-3P  
 RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation)  
 (esterase-activated two-**fluorophore** system for ratiometric  
 sensing of biol. zinc(II))

RN 615552-02-8 CAPLUS  
 CN Spiro[isobenzofuran-1(3H), 9' - [9H]xanthene] -6-carboxamide,  
 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
 dihydroxy-N-(4-hydroxybutyl)-3-oxo- (9CI) (CA INDEX NAME)



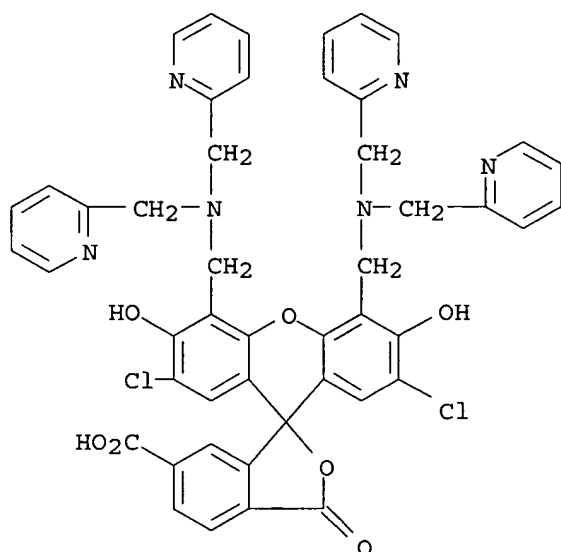
RN 616215-78-2 CAPLUS  
 CN Spiro[isobenzofuran-1(3H), 9' - [9H]xanthene] -6-carboxamide,  
 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
 dihydroxy-N-(2-hydroxyethyl)-3-oxo- (9CI) (CA INDEX NAME)





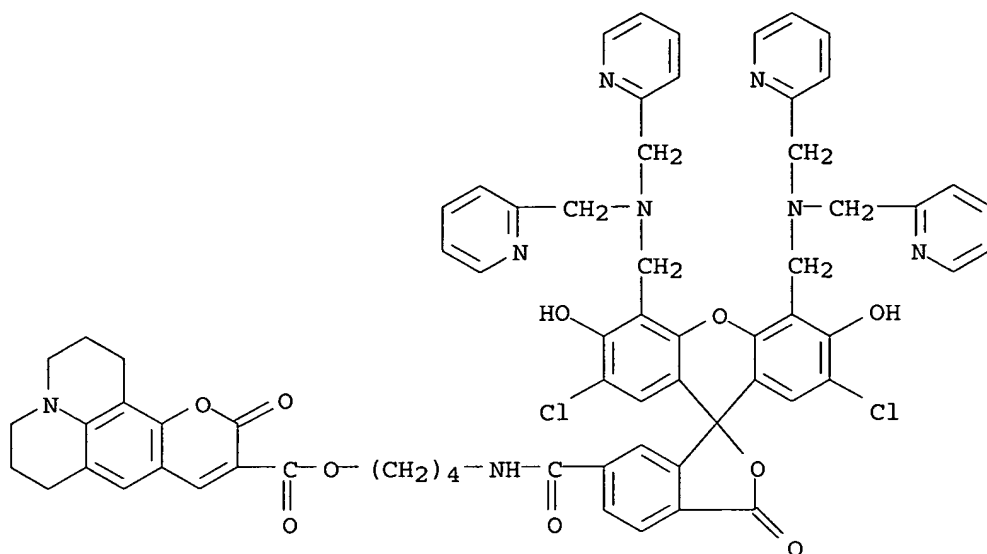
RN 790660-95-6 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9' - [9H]xanthene]-6-carboxylic acid,  
4', 5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2', 7'-dichloro-3', 6'-  
dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



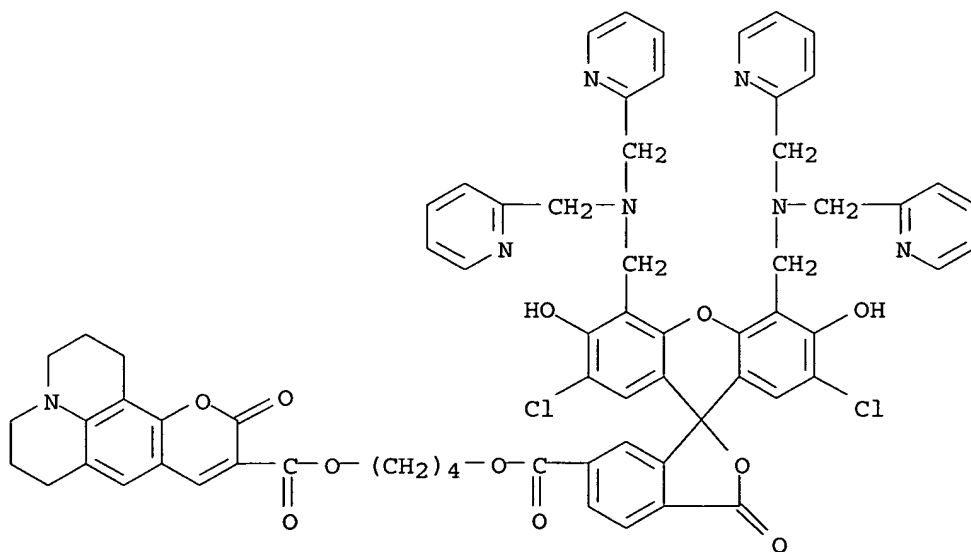
RN 852299-72-0 CAPLUS

CN 1H, 5H, 11H- [1]Benzopyrano[6, 7, 8-ij]quinolizine-10-carboxylic acid,  
2, 3, 6, 7-tetrahydro-11-oxo-, 4-[[[4', 5'-bis[[bis(2-  
pyridinylmethyl)amino]methyl]-2', 7'-dichloro-3', 6'-dihydroxy-3-  
oxospiro[isobenzofuran-1(3H), 9' - [9H]xanthene]-6-yl]carbonyl]amino]butyl  
ester (9CI) (CA INDEX NAME)



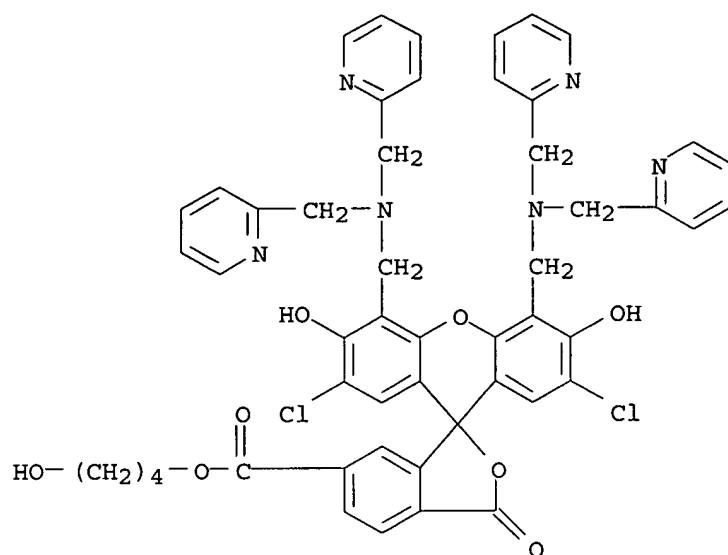
RN 852299-74-2 CAPLUS

CN 1H,5H,11H-[1]Benzopyrano[6,7,8-ij]quinolizine-10-carboxylic acid, 2,3,6,7-tetrahydro-11-oxo-, 4-[[[4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]oxy]butyl ester (9CI) (CA INDEX NAME)



RN 852299-75-3 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy-3-oxo-, 4-hydroxybutyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 10 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1089410 CAPLUS

DOCUMENT NUMBER: 142:459358

TITLE: Membrane-Permeable and -Impermeable Sensors of the Zinpyr Family and Their Application to Imaging of Hippocampal Zinc in Vivo

AUTHOR(S): Woodroffe, Carolyn C.; Masalha, Rafik; Barnes, Katie R.; Frederickson, Christopher J.; Lippard, Stephen J.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemistry & Biology (2004), 11(12), 1659-1666  
CODEN: CBOLE2; ISSN: 1074-5521

PUBLISHER: Cell Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Esterification of **fluorescent** biosensors is a common strategy used to trap probes within the **cell**. Zinpyr-1 (ZP1) is a **fluorescein**-based bright **fluorescent** sensor for divalent zinc that is **cell** permeable without prior modification. We describe here the synthesis and characterization of ZP1 sensors containing a carboxylic acid or Et ester functionality at the 5 or 6 position of the **fluorescein**. The presence of an electroneg. carboxylate decreases the proton-induced background **fluorescence** of the probe by lowering the pKa of the benzylic amines responsible for **fluorescence** quenching. The charged species ZP1(6-CO<sub>2</sub><sup>-</sup>) is membrane-impermeant, whereas the permeability of the neutral ZP1(5/6-CO<sub>2</sub>Et) is similar to that of the parent sensor. Intracranial microinfusion of ZP1(6-CO<sub>2</sub>Et) into rat hippocampus produces reduced staining of vesicular zinc in neuropil and very clear delineation of zinc-pos. injured neuronal somata and dendrites as compared with ZP1.

CC 9-1 (Biochemical Methods)

Section cross-reference(s): 13

IT Biosensors

Dendrite (neuron)

Esterification

Fluorescence quenching

Imaging

Neuron

Permeability

Rattus

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

IT 2321-07-5, **Fluorescein**

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

IT **288574-78-7P**, Zinpyr-1 502467-23-4P, Zinpyr 4

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

IT 142975-81-3 144316-86-9 144489-09-8 144489-10-1 790660-93-4

790660-94-5 **851620-50-3 851620-51-4****851620-52-5 851620-53-6**

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

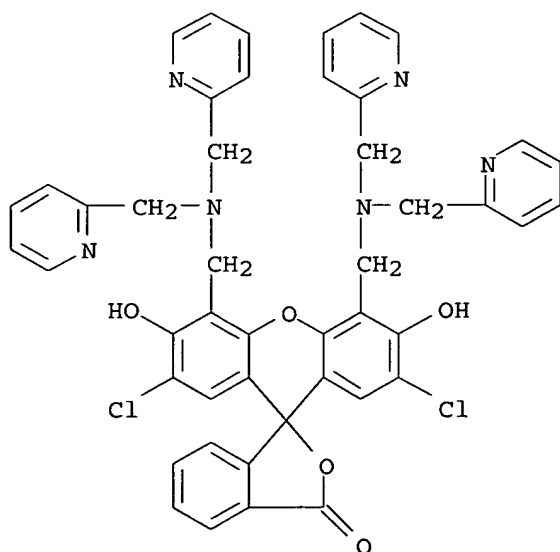
IT **288574-78-7P**, Zinpyr-1

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

IT **851620-50-3 851620-51-4 851620-52-5****851620-53-6**

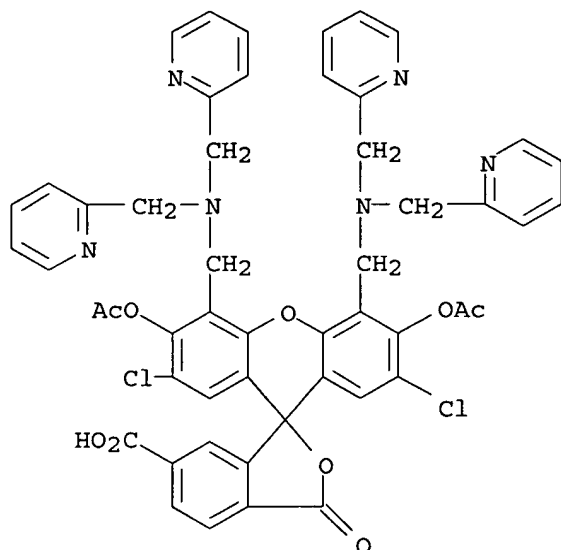
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation,

nonpreparative); RACT (Reactant or reagent)

(membrane-permeable and -impermeable sensors of zinpyr family and their application to imaging of hippocampal zinc in vivo)

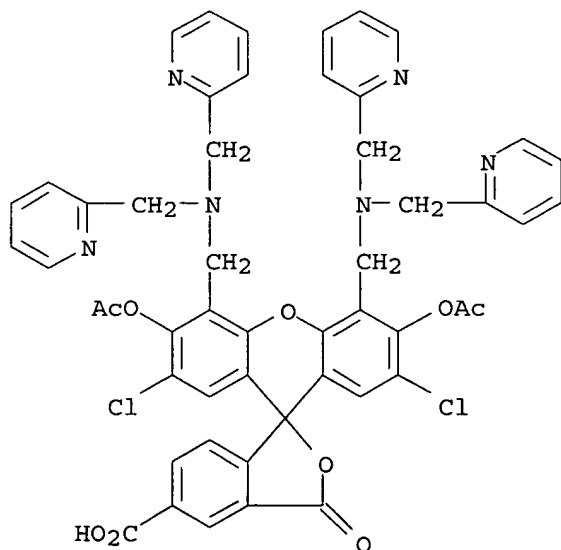
RN 851620-50-3 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,  
3',6'-bis(acetyloxy)-4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-  
dichloro-3-oxo- (9CI) (CA INDEX NAME)



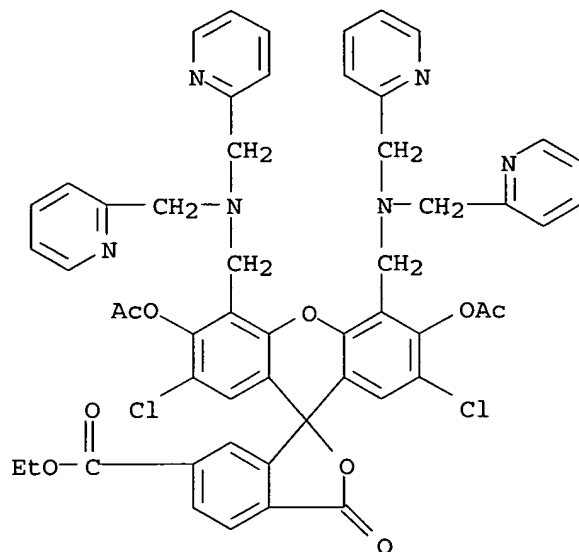
RN 851620-51-4 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid,  
3',6'-bis(acetyloxy)-4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-  
dichloro-3-oxo- (9CI) (CA INDEX NAME)



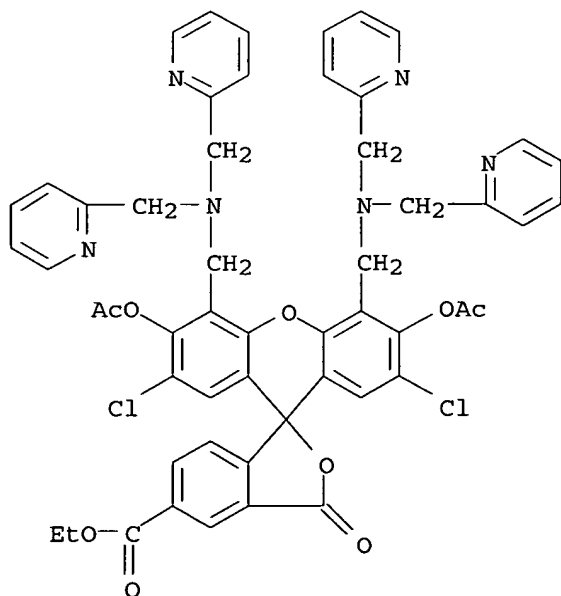
RN 851620-52-5 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,  
3',6'-bis(acetyloxy)-4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-  
dichloro-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 851620-53-6 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid,  
3',6'-bis(acetyloxy)-4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-  
dichloro-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 11 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:964729 CAPLUS  
 DOCUMENT NUMBER: 141:391502  
 TITLE: Sensors, and methods of making and using the same  
 INVENTOR(S): Lippard, Stephen J.; Woodrooffe, Carolyn Crystal  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 63 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE     |
|------------------------|------|----------|-----------------|----------|
| US 2004224420          | A1   | 20041111 | US 2003-429898  | 20030504 |
| PRIORITY APPLN. INFO.: |      |          | US 2003-429898  | 20030504 |

OTHER SOURCE(S): MARPAT 141:391502

AB The present invention is directed, in part, to sensors for detecting metal ions, and methods of making and using the same. **Fluorescence** technol. has revolutionized cell biol. and many areas of biochem. In certain instances, **fluorescent** mols. may be used to trace mol. and physiol. events in living cells. Certain sensitive and quant. **fluorescence** detection devices have made **fluorescence** measurements an ideal readout for in vitro biochem. assays. In addition **fluorescence** measurement systems may be useful for determining the presence of analytes in environmental samples. Finally, because certain **fluorescence** detection systems are rapid and reproducible, **fluorescence** measurements are often used in high-throughput screening applications. The feasibility of using **fluorescence** technol. for a particular application is often limited by the availability of an appropriate **fluorescent** sensor.

IC ICM G01N033-00

INCL 436074000

CC 9-1 (Biochemical Methods)

Section cross-reference(s): 14

IT Sensors

(**fluorometric**; sensors and methods of making and using the same)

IT Cations

Cell

Chemical formula

Diagnosis

**Fluorescence** quenching

**Fluorescent** substances

**Fluorometers**

**Fluorometry**

Human

Sensors

Test kits

(sensors and methods of making and using the same)

IT 67-68-5, DMSO, reactions 75-75-2, Methanesulfonic acid 76-54-0, 2',7'-**Dichlorofluorescein** 77-48-5 79-37-8, Oxalyl chloride 85-44-9, Phthalic anhydride 93-97-0, Benzoic anhydride 95-88-5, 4-Chlororesorcinol 107-06-2, 1,2-Dichloroethane, reactions 112-02-7, Cetyltrimethylammonium chloride 121-44-8, Triethylamine, reactions 288-32-4, Imidazole, reactions 446-33-3, 5-**Fluoro**-2-nitrotoluene 528-44-9, 1,2,4-Benzenetricarboxylic acid 536-90-3, m-Anisidine 608-25-3, 2-Methylresorcinol 1121-60-4, 2-Pyridinecarboxaldehyde 2094-98-6, 1,1'-Azobiscyclohexanecarbonitrile

2491-18-1 2706-56-1, 2-Aminoethylpyridine 3731-51-9,  
 2-Aminomethylpyridine 4377-33-7, Picolyl chloride 5367-28-2,  
 2-Nitro-5-chlorotoluene 5367-32-8, 3-Methyl-4-nitroanisole 6959-47-3,  
 Picolyl chloride hydrochloride 7446-70-0, Aluminum chloride (AlCl<sub>3</sub>),  
 reactions 27252-21-7, Benzenetricarboxylic acid 29227-68-7,  
 Dipicolylamine 30525-89-4, Paraformaldehyde 56553-60-7, Sodium  
 triacetoxyborohydride 144489-10-1 389625-48-3 479578-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(sensors and methods of making and using the same)

IT 2513-33-9P 31577-25-0P 67567-46-8P 111843-78-8P 118797-71-0P  
 144489-09-8P **288574-78-7P 357916-12-2P** 389625-45-0P  
 389625-46-1P 389625-47-2P 389625-49-4P 389625-50-7P 489469-65-0P  
 615552-00-6P 686767-82-8P 686767-84-0P 686767-86-2P 686767-87-3P,  
 Zinpyr-6 Imine 686767-89-5P, Zinpyr 5 686767-90-8P, Zinpyr 6  
 790660-90-1P 790660-91-2P 790660-93-4P 790660-94-5P  
**790660-95-6P 790660-96-7P 790660-97-8P**  
**790660-98-9P 790660-99-0P** 790661-00-6P 790661-01-7P  
 790661-02-8P 790661-04-0P 790661-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(sensors and methods of making and using the same)

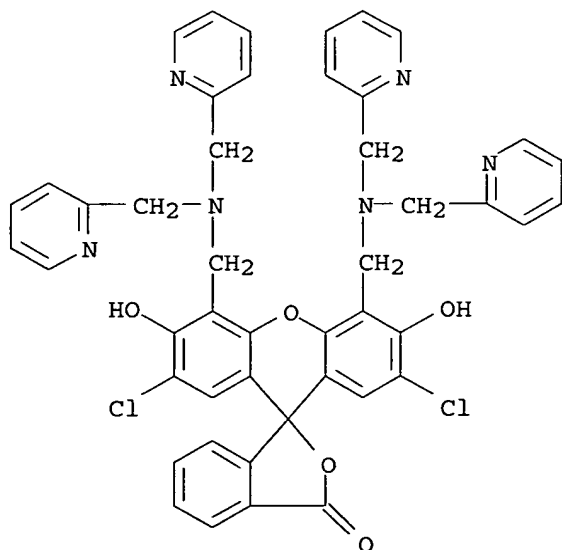
IT **288574-78-7P 357916-12-2P 790660-95-6P**  
**790660-96-7P 790660-97-8P 790660-98-9P**  
**790660-99-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(sensors and methods of making and using the same)

RN 288574-78-7 CAPLUS

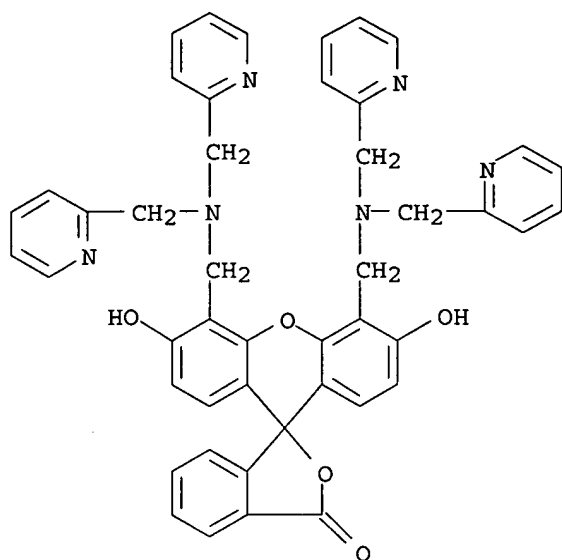
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



RN 357916-12-2 CAPLUS

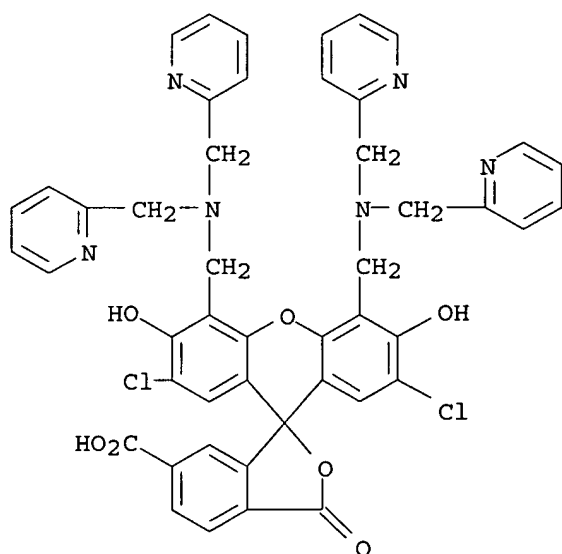
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)





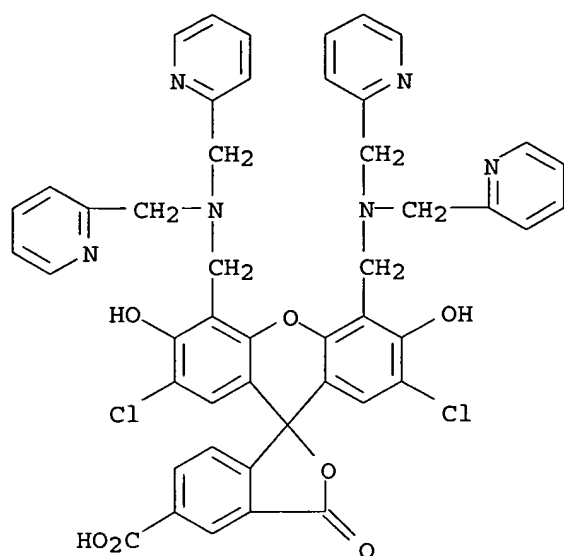
RN 790660-95-6 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthene]-6-carboxylic acid,  
4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



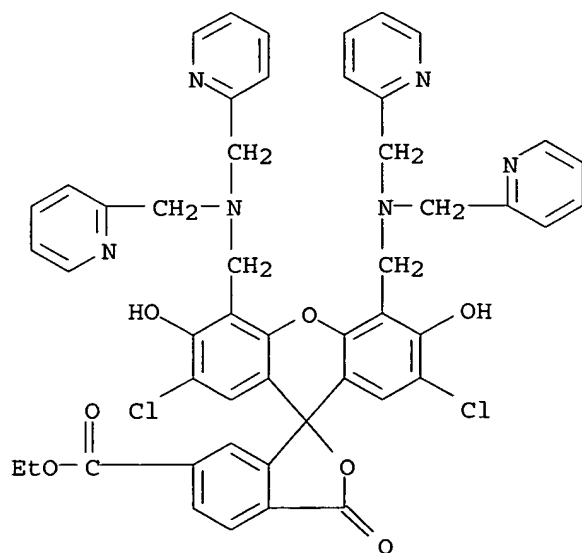
RN 790660-96-7 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthene]-5-carboxylic acid,  
4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



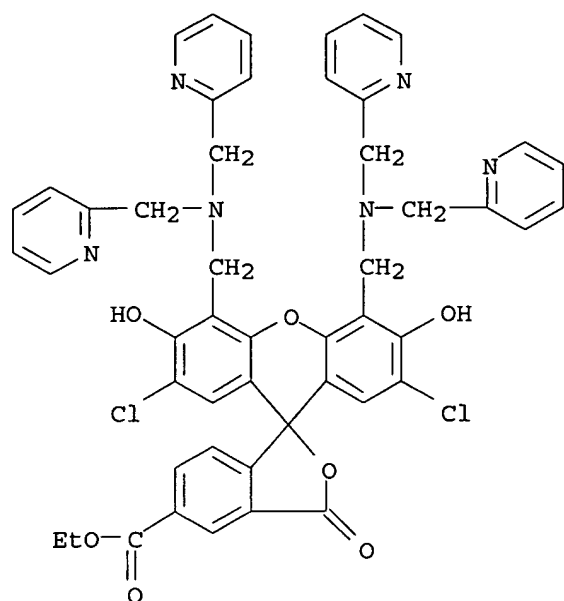
RN 790660-97-8 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthene]-6-carboxylic acid,  
4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
dihydroxy-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



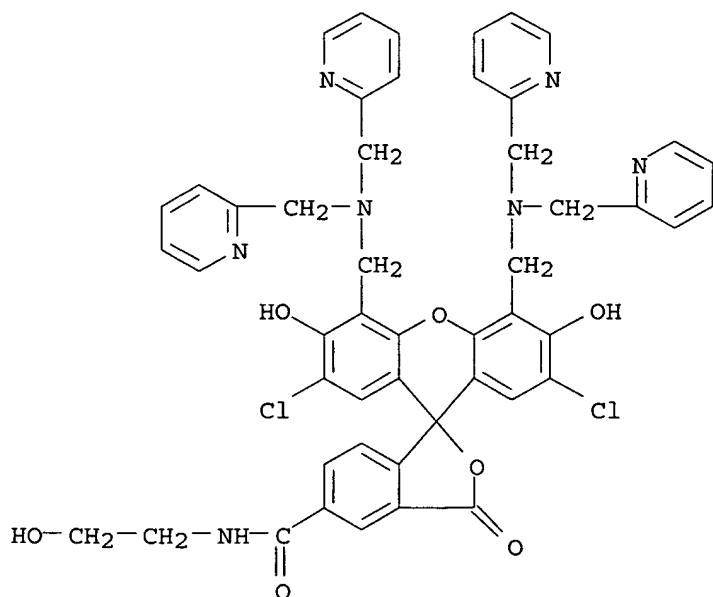
RN 790660-98-9 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthene]-5-carboxylic acid,  
4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
dihydroxy-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 790660-99-0 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9' - [9H]xanthene]-5-carboxamide,  
4',5'-bis[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-  
dihydroxy-N-(2-hydroxyethyl)-3-oxo- (9CI) (CA INDEX NAME)



L79 ANSWER 12 OF 52

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

CAPLUS COPYRIGHT 2006 ACS on STN

2004:927021 CAPLUS

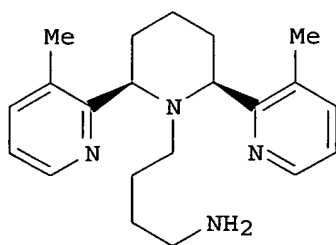
141:395421

Preparation of cis-2,6-di(pyridyl)piperidines and  
other cis-di(heteroaryl)-substituted azaheterocycles  
as binding agents for CXCR4 and other chemokine

receptors for treatment of HIV, rheumatoid arthritis,  
and other diseases and for stimulating progenitor and  
stem cells

INVENTOR(S): Bridger, Gary J.; McEachern, Ernest J.; Skerlj,  
Renato; Schols, Dominique  
PATENT ASSIGNEE(S): Anormed Inc., Can.  
SOURCE: PCT Int. Appl., 221 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO.   | DATE       |
|--|------|----------|-------------------|------------|
| WO 2004093817  | A2   | 20041104 | WO 2004-US12627   | 20040422   |
| WO 2004093817  | A3   | 20050428 |                   |            |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,<br>CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,<br>LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,<br>NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,<br>TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW<br>RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,<br>BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,<br>ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,<br>SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,<br>TD, TG |      |          |                   |            |
| AU 2004232361  | A1   | 20041104 | AU 2004-232361    | 20040422   |
| CA 2517077   | AA   | 20041104 | CA 2004-2517077   | 20040422   |
| EP 1615633   | A2   | 20060118 | EP 2004-760161    | 20040422   |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,<br>IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR   |      |          |                   |            |
| PRIORITY APPLN. INFO.:   |      |          | US 2003-464858P   | P 20030422 |
|  |      |          | US 2003-505230P   | P 20030922 |
|  |      |          | WO 2004-US12627   | A 20040422 |
| OTHER SOURCE(S):   |      |          | MARPAT 141:395421 |            |
| GI   |      |          |                   |            |



II

AB Cis-di(heteroaryl)-substituted azaheterocycle compds. A-C(B)-L-Y I [A, B = (un)substituted five- or six-membered heteroaryl moiety containing a nitrogen atom next to the bond to ring C; C = (un)substituted partially or fully saturated azaheterocycle with 5-8 ring atoms; L = (un)substituted alkanediyl, alkenediyl, alkynediyl; Y = H, (un)substituted alkyl which may contain heteroatoms, (un)substituted cyclic group; at least one of A or B must be substituted when C is either a piperidinyl or 1,2,3,6-tetrahydropyridinyl ring, and both A and B may not be substituted with naphthalenyl groups if

A and B are pyridinyl groups and if C is a piperidinyl moiety; if L-Y is Me, C is not 4-oxo-3,5-piperidinedicarboxylic acid, and if L-Y is benzyl, C is not a 4-hydroxy-1,2,5,6-tetrahydro-3-pyridinecarboxylic acid ester] such as II are prepared as agents capable of binding to chemokine receptors (particularly the CXCR4 receptor) for treatment of a variety of conditions such as HIV infection, cancer, inflammation, rheumatoid arthritis, immune system disorders, or diseases requiring stimulation of progenitor or stem **cells** for treatment. Lithium-bromine exchange of 2-bromo-3-methylpyridine followed by addition of the pyridyllithium to di-Me glutarate yields 1,5-bis(3-methyl-2-pyridinyl)-1,5-pentanedione; reduction of the dione with sodium borohydride in methanol to the dipyridinylpentanediol, dimesylation, substitution and cyclization with allylamine and separation of the cis- and trans-piperidines, palladium-mediated N-deallylation, alkylation of the piperidine nitrogen with 4-(N-phthalimidyl)-1-bromobutane, and hydrazine-mediated cleavage of the phthalimide yields II. Compds. I inhibit HIV replication with IC50 values between 0.5 nM and 5  $\mu$ M, and inhibit SDF-1 $\alpha$ -induced calcium flux with IC50 values between 0.5 nM and 5  $\mu$ M (no data). Compds. of the invention increase and mobilize mouse and human progenitor **cells**, increase white blood **cell** count in HIV-infected people, and mobilize CD34-pos. **cells** in humans; in addition, compds. of the invention mobilize bone marrow **cells** to repair heart muscle (no data).

IC ICM A61K

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

IT Chemokine receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(CXCR4; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem **cells**)

IT Anemia (disease)

(aplastic, treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases such as HIV)

IT Inflammation

(bacterial, treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases)

IT Interleukin 1

Interleukin 3

Interleukin 8

Macrophage inflammatory protein 1

Stem **cell** factor

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(codrug administered with cis-di(heteroaryl)-substituted azaheterocycle cytokine receptor binding agents for stimulation of progenitor or stem **cells** in treatment of diseases)

IT Anemia (disease)

(drug-induced, treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases)

IT Angiogenesis inhibitors

Bone marrow

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of

- progenitor or stem **cells** in treatment of diseases)
- IT Stem **cell**  
(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases such as HIV)
- IT Human  
(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem **cells**)
- IT Wound  
(treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases)
- IT Leukemia  
Leukocyte  
(treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of diseases such as HIV)
- IT Heart  
(treatment of; preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for stimulation of progenitor or stem **cells** in treatment of heart damage)
- IT 9014-42-0, Thrombopoietin 83869-56-1, GM-CSF 137463-76-4, PIXY-321 143011-72-7, G-CSF  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(codrug administered with cis-di(heteroaryl)-substituted azaheterocycle cytokine receptor binding agents for stimulation of progenitor or stem **cells** in treatment of diseases)
- IT 788087-94-5P 790273-61-9P  
RL: BYP (Byproduct); PREP (Preparation)  
(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem **cells**)
- IT 788062-91-9P  
RL: BYP (Byproduct); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem **cells**)
- IT 788061-59-6P 788061-65-4P 788062-75-9P 788063-62-7P 788063-85-4P  
788065-43-0P 788065-52-1P 788065-60-1P 788065-77-0P 788066-09-1P  
788066-16-0P 788066-38-6P 788066-52-4P 788068-58-6P 788070-79-1P  
788071-71-6P 788072-33-3P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem **cells**)
- IT 788061-73-4P 788061-81-4P 788061-89-2P 788061-95-0P 788062-04-4P  
788062-10-2P 788062-18-0P 788062-24-8P 788062-33-9P 788062-39-5P

|                     |              |              |              |              |
|---------------------|--------------|--------------|--------------|--------------|
| 788062-47-5P        | 788062-53-3P | 788062-61-3P | 788062-67-9P | 788062-82-8P |
| 788062-97-5P        | 788063-07-0P | 788063-13-8P | 788063-22-9P | 788063-29-6P |
| 788063-38-7P        | 788063-46-7P | 788063-54-7P | 788063-68-3P | 788063-77-4P |
| 788063-93-4P        | 788063-99-0P | 788064-08-4P | 788064-15-3P | 788064-25-5P |
| <b>788064-33-5P</b> | 788064-41-5P | 788064-50-6P | 788064-56-2P | .            |
| 788064-64-2P        | 788064-71-1P | 788064-80-2P | 788064-94-8P | 788065-00-9P |
| 788065-08-7P        | 788065-22-5P | 788065-28-1P | 788065-37-2P | 788065-69-0P |
| 788065-84-9P        | 788065-94-1P | 788066-00-2P | 788066-24-0P | 788066-30-8P |
| 788066-45-5P        | 788066-58-0P | 788066-68-2P | 788066-75-1P | 788066-84-2P |
| 788066-92-2P        | 788067-00-5P | 788067-10-7P | 788067-16-3P | 788067-24-3P |
| 788067-29-8P        | 788067-37-8P | 788067-43-6P | 788067-51-6P | 788067-58-3P |
| 788067-66-3P        | 788067-73-2P | 788067-83-4P | 788067-89-0P | 788067-98-1P |
| 788068-05-3P        | 788068-13-3P | 788068-26-8P | 788068-33-7P | 788068-42-8P |
| 788068-48-4P        | 788068-66-6P | 788068-73-5P | 788068-83-7P | 788068-88-2P |
| 788068-94-0P        | 788069-02-3P | 788069-11-4P | 788069-17-0P | 788069-26-1P |
| 788069-33-0P        | 788069-41-0P | 788069-46-5P | 788069-54-5P | 788069-61-4P |
| 788069-70-5P        | 788069-76-1P | 788069-85-2P | 788069-91-0P | 788069-99-8P |
| 788070-04-2P        | 788070-13-3P | 788070-19-9P | 788070-28-0P | 788070-35-9P |
| 788070-44-0P        | 788070-50-8P | 788070-57-5P | 788070-64-4P | 788070-73-5P |
| 788070-88-2P        | 788070-95-1P | 788071-02-3P | 788071-08-9P | 788071-16-9P |
| 788071-23-8P        | 788071-32-9P | 788071-38-5P | 788071-47-6P | 788071-56-7P |
| 788071-63-6P        | 788071-77-2P | 788071-85-2P | 788071-93-2P | 788072-02-6P |
| 788072-08-2P        | 788072-17-3P | 788072-24-2P | 790273-50-6P | 790273-51-7P |
| 790273-52-8P        |              |              |              |              |

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem cells)

IT 77-77-0, Divinyl sulfone 89-71-4, Methyl 2-methylbenzoate 95-54-5, 1,2-Phenylenediamine, reactions 96-32-2, Methyl bromoacetate 96-98-0, 4-Methyl-3-nitrobenzoic acid 98-09-9, Benzenesulfonyl chloride 98-59-9, p-Toluenesulfonyl chloride 100-11-8, 4-Nitrobenzyl bromide 106-95-6, Allyl bromide, reactions 107-11-9, Allylamine 109-64-8, 1,3-Dibromopropane 123-75-1, Pyrrolidine, reactions 127-06-0, Acetone oxime 288-32-4, Imidazole, reactions 452-74-4, 1-Bromo-2-fluoro-4-methylbenzene 542-05-2, 1,3-Acetonedicarboxylic acid 577-16-2, 2'-Methylacetophenone 623-24-5, 1,4-Bis(bromomethyl)benzene 1074-82-4, Potassium phthalimide 1118-02-1, Trimethylsilyl isocyanate 1119-40-0, Dimethyl glutarate 1121-60-4, 2-Pyridinecarboxaldehyde 2042-14-0, 4-Methyl-3-nitrophenol 2417-72-3, Methyl 4-(bromomethyl)benzoate 2687-43-6, O-Benzylhydroxylamine hydrochloride 3251-69-2, 4-Imidazoleacetic acid hydrochloride 3332-29-4, O-Ethylhydroxylamine hydrochloride 3430-17-9, 2-Bromo-3-methylpyridine 3556-83-0, Methyl 3-methoxy-4-methylbenzoate 3581-89-3, 5-Methylthiazole 3893-01-4, 2,3-Dimethoxybenzyl chloride 3958-60-9, 2-Nitrobenzyl bromide 4009-98-7, **Methoxymethyltriphenylphosphonium** chloride 4286-15-1, (S)-2-Phenylbutyric acid 5006-62-2, Ethyl nipecotate 5006-66-6, 6-Hydroxynicotinic acid 5332-06-9, 4-Bromobutyronitrile 5394-18-3, 2-(4-Bromobutyl)isoindole-1,3-dione 7035-02-1, 2-Methoxybenzyl chloride 7040-23-5 10111-08-7, 2-Imidazolecarboxaldehyde 13518-55-3, 4-(2-Chloroethyl)imidazole 13958-93-5, 3,5-Dichloro-4-pyridinecarboxylic acid 14660-52-7, Ethyl 5-bromopentanoate 17201-43-3,  $\alpha$ -Bromo-p-tolunitrile 18226-11-4 20970-75-6, 3-Methylpicolinonitrile 22115-41-9,  $\alpha$ -Bromo-o-tolunitrile 25542-62-5, Ethyl 6-bromohexanoate 28188-41-2,  $\alpha$ -Bromo-m-tolunitrile 31106-82-8, 2-(Bromomethyl)pyridine hydrobromide 32673-41-9, 4-(Hydroxymethyl)imidazole hydrochloride

33184-16-6, 5-**Fluoro**-2-methylbenzoic acid 39931-77-6, Ethyl  
 3-pyridylacetate 40473-30-1 42383-61-9, 2-Aminoimidazole sulfate  
 55589-47-4, 3-Methyl-2-pyridinecarboxaldehyde 58885-60-2,  
 3-(tert-Butoxycarbonylamino)propanal 63874-95-3, 1-Benzyl-4-  
 pyrazolecarboxaldehyde 68076-36-8, (4-Aminobutyl)carbamic acid  
 tert-butyl ester 73870-24-3, 4-(Bromomethyl)pyridine hydrobromide  
 80263-42-9, 3-Isopropyl-2-methylpyridine 85684-64-6, 2-(  
**Difluoromethoxy**)benzyl bromide 88811-36-3, 4-(3-  
 Hydroxypropyl)imidazole-1-carboxylic acid tert-butyl ester 99207-32-6  
 99708-91-5, 4-(Bromomethyl)-3-thiophenecarbonitrile 103261-68-3, Methyl  
 5-cyano-2-methylbenzoate 123642-28-4 132873-77-9, 4-(Bromomethyl)-1-  
 benzimidazolecarboxylic acid tert-butyl ester 202932-05-6 206181-90-0,  
 3-Chloro-2-pyridinecarboxaldehyde 255383-17-6 325775-44-8, tert-Butyl  
 3-(aminomethyl)-1-azetidinecarboxylate 421551-82-8, Methyl  
 2-(bromomethyl)-5-cyanobenzoate 780801-55-0, 5-Chloro-3-methyl-2-  
 pyridinecarboxaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding  
 agents for CXCR4 and other chemokine receptors for treatment of HIV,  
 rheumatoid arthritis and other diseases and for stimulation of  
 progenitor or stem cells)

IT 103-74-2P, 2-(2-Pyridinyl)ethanol 2417-73-4P, Methyl  
 2-bromomethylbenzoate 4200-46-8P 5460-29-7P 5664-55-1P,  
 5-Thiazoleethanol 7356-11-8P, Methyl 4-methyl-3-nitrobenzoate  
 7720-39-0P, 2-Aminoimidazole 16281-94-0P, Dimethyl 4-  
 bromomethylisophthalate 17484-36-5P, 4-Methoxy-1-methyl-2-nitrobenzene  
 18595-18-1P, Methyl 3-amino-4-methylbenzoate 22246-19-1P,  
 5-Methoxy-2-methylbenzonitrile 23038-61-1P, Dimethyl  
 4-methylisophthalate 35066-32-1P, Methyl 3-cyano-4-methylbenzoate  
 37709-53-8P 50382-34-8P, 5-Thiazoleacetonitrile 50868-72-9P,  
 5-Methoxy-2-methylaniline 70264-94-7P, Methyl 4-bromomethyl-3-  
 methoxybenzoate 73502-03-1P 73505-48-3P 85070-67-3P, 2-  
**Fluoro**-4-methylbenzonitrile 88089-94-5P 88811-37-4P  
 94614-83-2P 99230-20-3P 116986-13-1P 121688-31-1P 138428-37-2P  
 138786-65-9P, Methyl 2-bromomethyl-5-**fluorobenzoate**  
 144385-79-5P 150982-68-6P 150982-69-7P 155742-57-7P 155742-58-8P  
 175278-29-2P, Methyl 5-**fluoro**-2-methylbenzoate 177940-27-1P  
 191982-64-6P 215871-21-9P 219519-17-2P 222978-03-2P,  
 4-Bromomethyl-2-**fluorobenzonitrile** 297180-07-5P 344951-08-2P  
 496921-42-7P 582299-09-0P 675138-02-0P 780800-72-8P 780800-73-9P  
 780800-74-0P 788072-39-9P 788072-48-0P 788072-54-8P 788072-63-9P  
 788072-72-0P 788072-78-6P 788072-87-7P 788072-93-5P 788073-01-8P  
 788073-08-5P 788073-16-5P 788073-23-4P 788073-31-4P 788073-38-1P  
 788073-46-1P 788073-51-8P 788073-59-6P 788073-66-5P 788073-74-5P  
 788073-80-3P 788073-89-2P 788073-95-0P 788074-04-4P 788074-11-3P  
 788074-18-0P 788074-24-8P 788074-31-7P 788074-40-8P 788074-48-6P  
 788074-62-4P 788074-68-0P 788074-93-1P 788075-02-5P 788075-09-2P  
 788075-18-3P 788075-31-0P 788075-45-6P 788075-51-4P 788075-65-0P  
 788075-73-0P 788075-80-9P 788075-88-7P 788076-08-4P 788076-22-2P  
 788076-31-3P 788076-39-1P 788076-46-0P 788076-54-0P 788076-61-9P  
 788076-70-0P 788076-77-7P 788076-90-4P 788077-12-3P 788077-18-9P  
 788077-27-0P 788077-50-9P 788077-57-6P 788077-66-7P 788077-72-5P  
 788077-80-5P 788077-86-1P 788077-95-2P 788078-01-3P 788078-08-0P  
 788078-15-9P 788078-53-5P 788078-63-7P 788078-68-2P 788078-76-2P  
 788079-02-7P 788079-09-4P 788079-16-3P 788079-23-2P 788079-31-2P  
 788079-37-8P 788079-50-5P 788079-59-4P 788079-65-2P 788079-72-1P  
 788079-80-1P 788079-94-7P 788080-02-4P 788080-21-7P 788080-29-5P  
 788080-35-3P 788080-42-2P 788080-49-9P 788080-57-9P 788080-64-8P  
 788080-77-3P 788080-98-8P 788081-04-9P 788081-11-8P 788081-27-6P  
 788081-32-3P 788081-59-4P 788081-68-5P 788081-74-3P 788081-99-2P



788082-07-5P 788082-26-8P 788082-34-8P 788082-53-1P 788082-62-2P  
 788082-68-8P 788082-77-9P 788082-90-6P 788083-02-3P 788083-09-0P  
 788083-17-0P 788083-23-8P 788083-31-8P 788083-38-5P 788083-46-5P  
 788083-60-3P 788083-73-8P 788083-79-4P 788084-05-9P 788084-24-2P  
 788084-32-2P 788084-40-2P 788084-47-9P 788084-56-0P 788084-61-7P  
 788084-75-3P 788084-83-3P 788084-89-9P 788084-99-1P 788085-06-3P  
 788085-14-3P 788085-37-0P 788085-46-1P 788085-67-6P 788085-78-9P  
 788085-89-2P 788085-99-4P 788086-10-2P 788086-18-0P 788086-32-8P  
 788086-43-1P 788086-50-0P 788088-03-9P 788088-09-5P 788088-16-4P  
 790273-53-9P 790273-54-0P 790273-55-1P 790273-56-2P 790273-57-3P  
 790273-58-4P 790273-59-5P 790273-60-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem cells)

IT 788088-38-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem cells)

IT 788064-33-5P

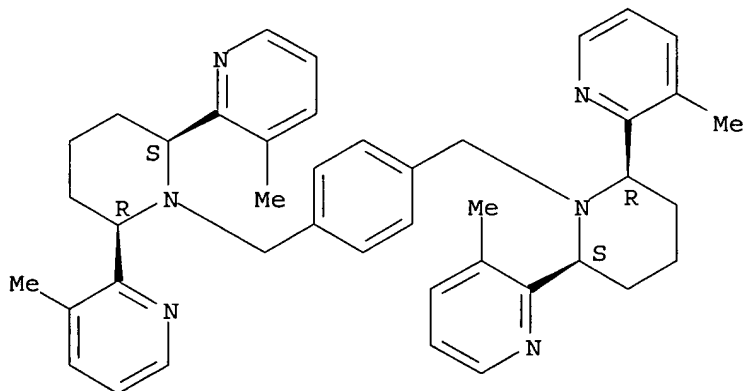
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other chemokine receptors for treatment of HIV, rheumatoid arthritis and other diseases and for stimulation of progenitor or stem cells)

RN 788064-33-5 CAPLUS

CN Pyridine, 2,2',2'',2'''-[1,4-phenylenebis(methylene-(2R,6S)-1,2,6-piperidinetriyl)]tetrakis[3-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L79 ANSWER 13 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

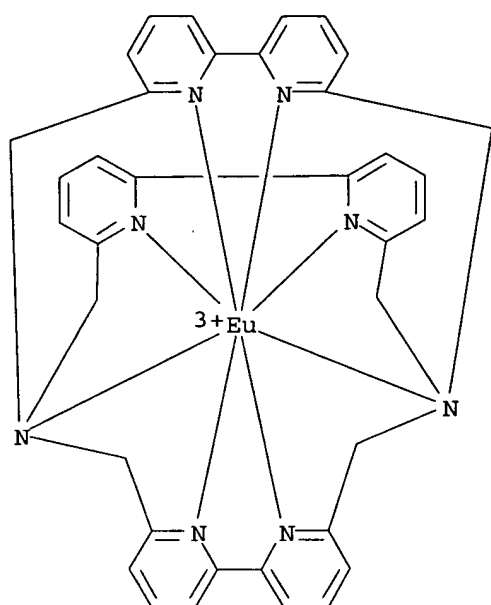
ACCESSION NUMBER: 2004:827855 CAPLUS

DOCUMENT NUMBER: 143:70385

TITLE: The sensitivity of the Lehn cryptand-europium and terbium(III) complexes to anions compared to a coordinatively saturated systems

AUTHOR(S): Cross, Jason P.; Dadabhoy, Anjum; Sammes, Peter G.  
 CORPORATE SOURCE: Department of Chemistry, School of Biological  
 Sciences, University of Surrey, Surrey, GU2 7XH, UK  
 SOURCE: Journal of Luminescence (2004), 110(3), 113-124  
 CODEN: JLUMA8; ISSN: 0022-2313  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

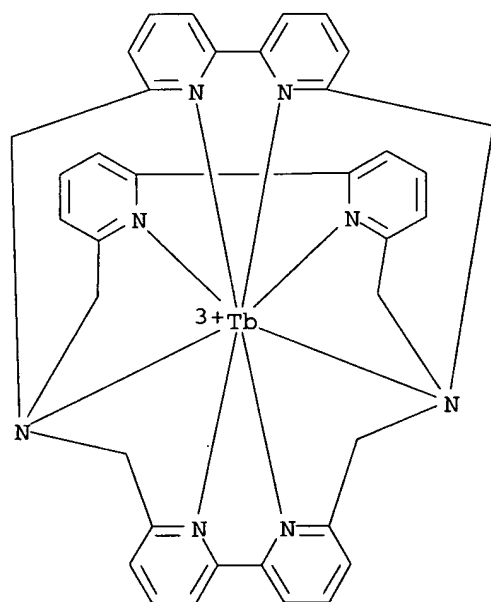
AB Titns. of the Lehn cryptand [Ln c bpy.bpy.bpy]3+ complexes of both  
 europium(III) and terbium(III) with **fluoride** and  
**phosphate** ions indicate that these anions displace water from the  
 solvation sphere. In the case of the europium complex an enhancement of  
 luminescence intensity is observed, while with the terbium complex a reduction  
 in  
 the emission intensity occurs. Described are the preps. of analogous,  
 coordinatively saturated complexes that are inert to the influence of these  
 anions.  
 CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 73  
 ST Lehn cryptand europium terbium prepn luminescence **fluoride**  
**phosphate**; rare earth bipyridylmethyl  
 tetraazacyclododecanetriacetate prepn luminescence  
 IT 854143-12-7P 854143-13-8P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and luminescence and effect of added **fluoride** and  
**phosphate**)  
 IT 134055-00-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of europium and terbium complexes with Lehn  
 cryptand)  
 IT 854143-12-7P 854143-13-8P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and luminescence and effect of added **fluoride** and  
**phosphate**)  
 RN 854143-12-7 CAPLUS  
 CN Europium(3+), (1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12  
 .116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,2  
 0(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-  
 κN1,κN14,κN39,κN40,κN41,κN42,κN4  
 3,κN44)-, trichloride, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



● 3 Cl<sup>-</sup>

RN 854143-13-8 CAPLUS

CN Terbium(3+), (1,14,39,40,41,42,43,44-octaazaocyclotetradeca-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-κN1,κN14,κN39,κN40,κN41,κN42,κN43,κN44)-, trichloride, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)



● 3 Cl<sup>-</sup>

IT 134055-00-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant for preparation of europium and terbium complexes with Lehn cryptand)

RN 134055-00-8 CAPLUS

CN Sodium(1+), (1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.16,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-  
κN1,κN14,κN39,κN40,κN41,κN42,κN43,κN44)-, bromide, (TPT-8-22'-11'11'11')- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 14 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:822093 CAPLUS

DOCUMENT NUMBER: 143:141619

TITLE: Spectroscopic properties of porphyrins and effect of lanthanide ions on their luminescence efficiency

AUTHOR(S): Wiglusz, R.; Legendziewicz, J.; Graczyk, A.; Radzki, S.; Gawryszewska, P.; Sokolnicki, J.

CORPORATE SOURCE: Faculty of Chemistry, University of Wroclaw, Wroclaw, 50-383, Pol.

SOURCE: Journal of Alloys and Compounds (2004), 380(1-2), 396-404

CODEN: JALCEU; ISSN: 0925-8388

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Spectroscopic properties of H2TPP porphyrin and Tb(III)TPP(acac) in solid and methanolic solns. were compared. Emission from the S1 singlet state of Tb(III)TPP(acac) were recorded at 296 and 77 K Spectroscopic studies of new types of porphyrins soluble in organic solvents (e.g. MeOH), PP(AA)2, and porphyrins soluble in H2O, PP(AA)2(Arg)2 (AA, alanine or **serine**; Arg, arginine), are presented. Interaction of PP(AA)2 with lanthanide ions (Yb(III), Eu(III)) was studied. The lanthanide (III) ions decrease efficiency of the porphyrin emission. For the alanine derivative, the stronger losses are caused by the Eu(III) ions as compared to the Yb(III) ions. However, the emission quenching by both lanthanide ions is similar in the case of the **serine** derivative Influence of the Pr(III) and Eu(III) ions on the PP(AA)2(Arg)2 emission also was studied. An unexpected increase of the porphyrin emission intensity was observed in solution

for the lowest concentration of Pr(III) added, whereas the Eu(III) ions quench the emission in the full range of its concentration The observed phenomena are analyzed, and the mechanisms of the excited-state dynamics in which the f-excited states take part in the porphyrin emission quenching are considered. The lanthanide ions influence the absorption spectrum as well as the relative intensities of the resp. bands in the emission spectra. The luminescence intensities of these porphyrins as a function of pH, the concentration and the type of the porphyrin substituent were analyzed. Significant influence of the above factors on the emission properties of the porphyrins was found and discussed. Efficiency of the emission was determined for these M-porphyrin systems in comparison to the free porphyrins in MeOH solns. The observed effects can be explained by formation of polymeric chains and decrease of face-to-face agglomeration that leads to effective quenching.

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 77

IT 917-23-7 7440-10-0D, Praseodymium, porphyrins complexes 7440-53-1D, Europium, porphyrins complexes 69458-20-4 849771-18-2 849771-20-6 849771-22-8 849771-23-9

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP

(Physical process); PROC (Process)

(Spectroscopic properties of porphyrins and effect of lanthanide ions on their luminescence efficiency)

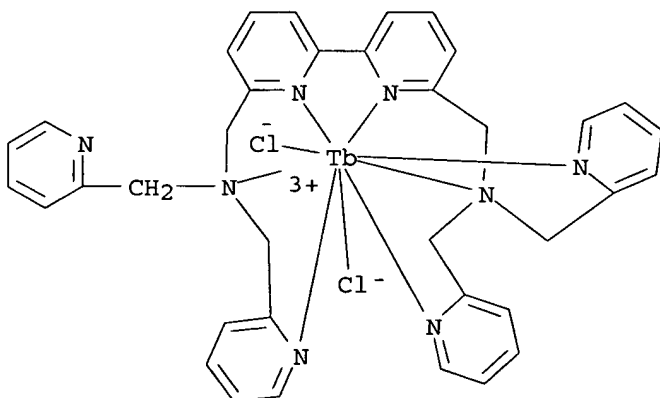
IT 849771-23-9

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(Spectroscopic properties of porphyrins and effect of lanthanide ions on their luminescence efficiency)

RN 849771-23-9 CAPLUS

CN Terbium(1+), dichloro[N,N,N'-tris[(2-pyridinyl-κN)methyl]-N'-(2-pyridinylmethyl)[2,2'-bipyridine]-6,6'-dimethanamine-κN1,κN1',κN6,κN6']-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 15 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:805193 CAPLUS

DOCUMENT NUMBER: 141:408097

TITLE: **Fluorescent sensors: A fluorescent pyrophosphate sensor with high selectivity over ATP in water**

AUTHOR(S): Lee, Dong Hoon; Kim, Soon Young; Hong, Jong-In  
CORPORATE SOURCE: Department of Chemistry, College of Natural Sciences, Seoul National University, Seoul, 151-747, S. Korea

SOURCE: Angewandte Chemie, International Edition (2004), 43(36), 4777-4780

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH &amp; Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:408097

AB High affinity and selective detection for PPI is exhibited by a new **fluorescent** sensor based on a naphthalene-dpa system. The binuclear zinc complex is remarkably selective toward PPI over other anions. For example, PPI can be detected at micromolar concns. in the presence of a large excess of ATP. PPI = **pyrophosphate**, ATP =

ATP, dpa = bis(2-pyridylmethyl)amine.

CC 9-5 (Biochemical Methods)

ST **fluorescence** sensor **pyrophosphate** high selectivity ATP  
water

IT Emission spectrometry

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

IT Sensors

(**fluorometric; fluorescent pyrophosphate**  
sensor with high selectivity over ATP in water)

IT 56-65-5, 5'-ATP, analysis

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
study); BIOL (Biological study)

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

IT **792959-43-4P** 792959-44-5P **793687-35-1P**

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

IT 1539-42-0 14221-01-3 32316-92-0, Boronic acid, 2-naphthalenyl-  
52113-69-6 206879-83-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

IT 792959-45-6P 792959-47-8P 792959-49-0P 792959-50-3P 792959-51-4P  
792959-52-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

IT 848938-34-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

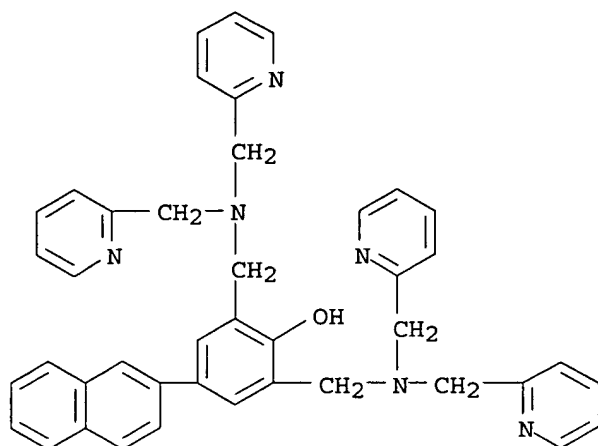
IT **792959-43-4P** **793687-35-1P**

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)

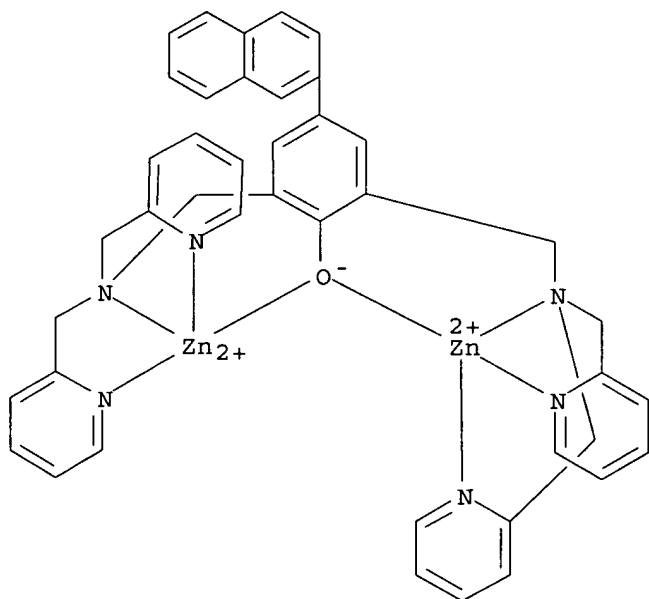
(**fluorescent pyrophosphate** sensor with high  
selectivity over ATP in water)

RN 792959-43-4 CAPLUS

CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-(2-naphthalenyl)-  
(9CI) (CA INDEX NAME)



RN 793687-35-1 CAPLUS  
 CN Zinc(3+), [ $\mu$ -[2,6-bis[[bis[(2-pyridinyl- $\kappa$ N)methyl]amino- $\kappa$ N)methyl]-4-(2-naphthalenyl)phenolato- $\kappa$ O: $\kappa$ O]]di- (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 16 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:749166 CAPLUS

DOCUMENT NUMBER: 141:408009

TITLE: ZP8, a Neuronal Zinc Sensor with Improved Dynamic Range; Imaging Zinc in Hippocampal Slices with Two-Photon Microscopy

AUTHOR(S): Chang, Christopher J.; Nolan, Elizabeth M.; Jaworski, Jacek; Okamoto, Kenichi; Hayashi, Yasunori; Sheng, Morgan; Lippard, Stephen J.

CORPORATE SOURCE: Department of Chemistry, Picower Center for Learning and Memory, RIKEN-MIT Neuroscience Research Center, and Howard Hughes Medical Institute, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Inorganic Chemistry (2004), 43(21), 6774-6779  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of a **difluorofluorescein** monocarboxaldehyde platform and its use for preparing ZP8, a new member of the Zinpyr family of neuronal Zn<sup>2+</sup> sensors, are described. By combining an aniline photoinduced electron transfer (PET) switch and an electron-withdrawing **fluorescein** scaffold, ZP8 displays reduced background **fluorescence** and improved dynamic range compared to previous ZP probes. The bright sensor undergoes an 11-fold increase in **fluorescence** intensity upon Zn<sup>2+</sup> complexation ( $\Phi = 0.03-0.35$ ) with high selectivity over **cellular** concns. of Ca<sup>2+</sup> and Mg<sup>2+</sup>. In addition, sensors in the ZP family have been utilized for optical imaging in biol. samples using two-photon microscopy (TPM). The **cell**-permeable ZP3 probe is capable of identifying natural pools of labile Zn<sup>2+</sup> within the mossy fiber synapses of live hippocampal slices using TPM, establishing the application of this technique for monitoring endogenous Zn<sup>2+</sup> stores.

CC 9-4 (Biochemical Methods)  
Section cross-reference(s): 13, 14

IT **288574-78-7**, ZP 1  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(Zinpyr 1; imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

IT **357916-12-2**, ZP 2  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(Zinpyr 2; imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

IT **791072-81-6**, ZP 3  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(Zinpyr 3; imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

IT 77-48-5 85-44-9, Phthalic anhydride 608-25-3, 2-Methyl resorcinol 103068-41-3, 4-**Fluororesorcinol** 140681-55-6 502467-17-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(imaging zinc in hippocampal slices with two-photon microscopy using ZP8, neuronal zinc biosensor)

IT 479578-63-7P, 2-Methyl-4-**fluororesorcinol** 479578-64-8P 790675-75-1P 790675-76-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(imaging zinc in hippocampal slices with two-photon microscopy using ZP8, neuronal zinc biosensor)

IT **791072-82-7**, ZPF 1 **791072-83-8**, ZPCl 1 **791072-84-9**, ZPBr 1 **791072-85-0**, ZPF 3  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)



(imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

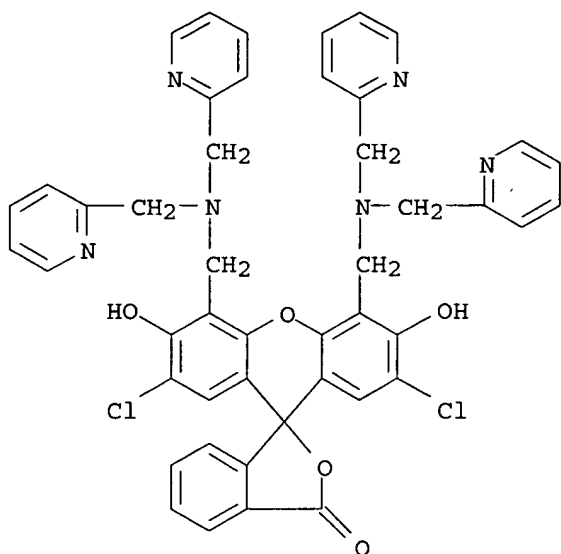
IT 288574-78-7, ZP 1

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(Zinpyr 1; imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



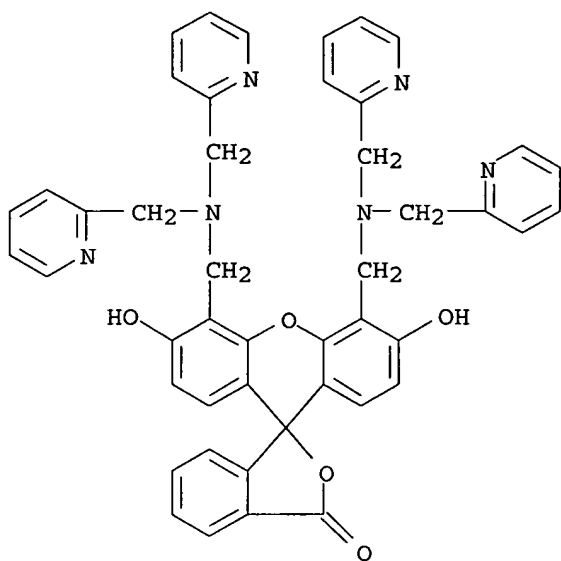
IT 357916-12-2, ZP 2

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)

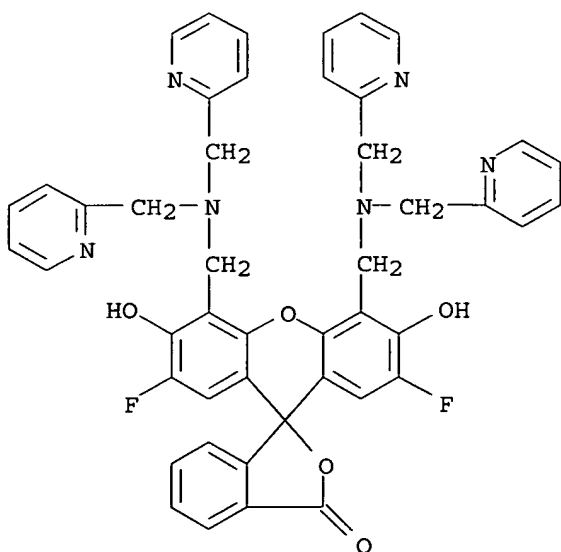
(Zinpyr 2; imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

RN 357916-12-2 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



IT 791072-81-6, ZP 3  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
 PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES  
 (Uses)  
 (Zinpyr 3; imaging zinc in hippocampal slices with two-photon  
 microscopy using neuronal zinc biosensor)  
 RN 791072-81-6 CAPLUS  
 CN Spiro[isobenzofuran-1(3H), 9']-[9H]xanthen-3-one, 4',5'-bis[[bis(2-  
 pyridinylmethyl)amino]methyl]-2',7'-difluoro-3',6'-dihydroxy- (9CI) (CA  
 INDEX NAME)



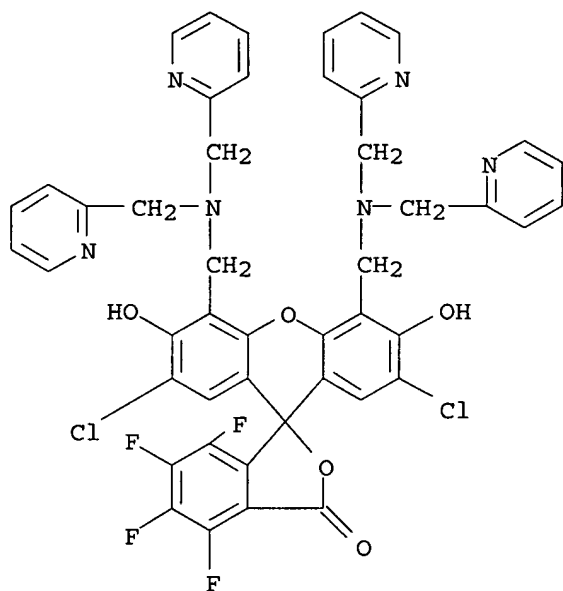
IT 791072-82-7, ZPF 1 791072-83-8, ZPCl 1  
 791072-84-9, ZPBr 1 791072-85-0, ZPF 3  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(imaging zinc in hippocampal slices with two-photon microscopy using neuronal zinc biosensor)

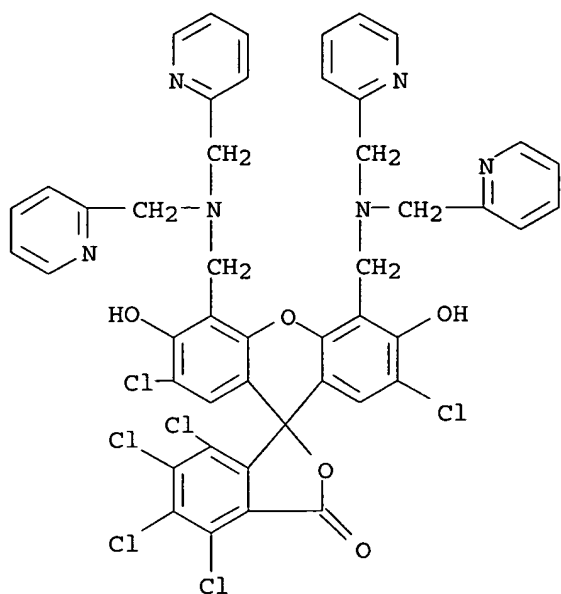
RN 791072-82-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9' - [9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-4,5,6,7-tetrafluoro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



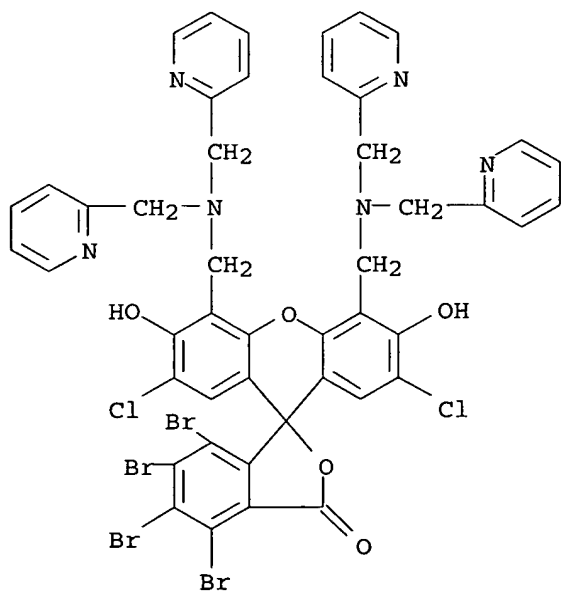
RN 791072-83-8 CAPLUS

CN Spiro[isobenzofuran-1(3H),9' - [9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',4,5,6,7,7'-hexachloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



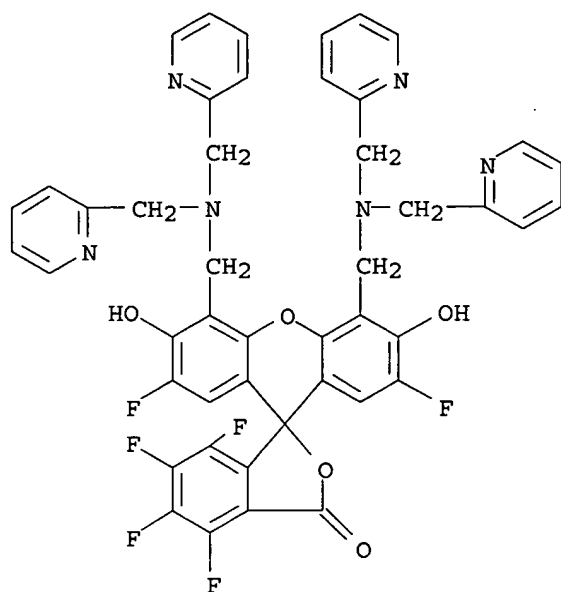
RN 791072-84-9 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-4,5,6,7-tetrachloro-2',7'-dihydroxy- (9CI) (CA INDEX NAME)



RN 791072-85-0 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',4,5,6,7,7'-hexafluoro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 17 OF 52 CAPLUS-- COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:735455 CAPLUS

DOCUMENT NUMBER: 141:407614

TITLE: A homogeneous time-resolved **fluorescence** detection of telomerase activity

AUTHOR(S): Gabourdes, Manuel; Bourguine, Valerie; Mathis, Gerard; Bazin, Herve; Alpha-Bazin, Beatrice

CORPORATE SOURCE: HTRF/Bioassays, CIS Bio International, Bagnols-sur-Ceze, F-30204, Fr.

SOURCE: Analytical Biochemistry (2004), 333(1), 105-113

CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Elsevier

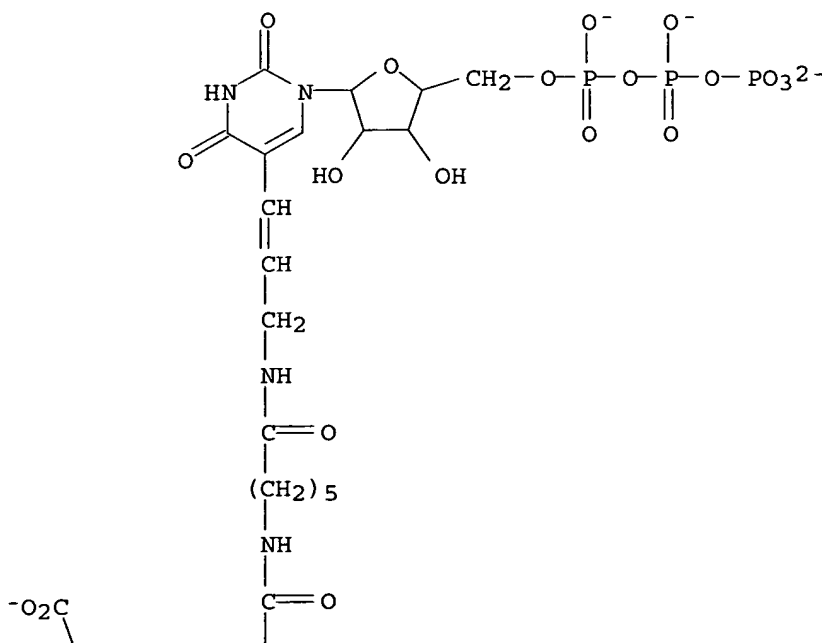
DOCUMENT TYPE: Journal

LANGUAGE: English

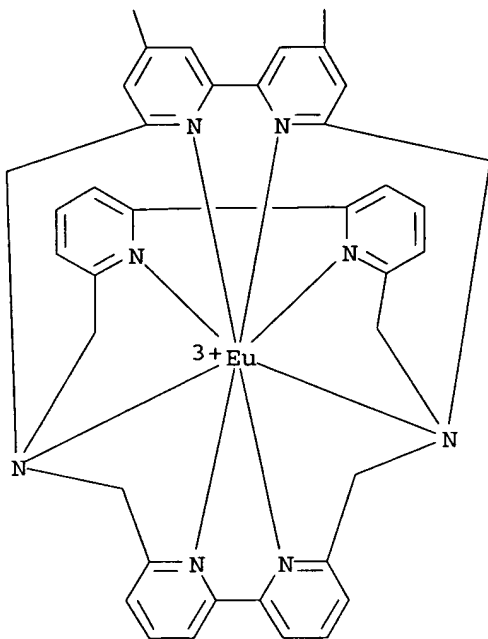
AB The homogeneous time-resolved **fluorescence** (HTRF) technol. is an assay developed to study the interaction between biomols. This detection system is based on a **fluorescence** resonance energy transfer (FRET) between a Tris-bipyridine europium cryptate used as a long-lived **fluorescent** donor and a chemical modified allophycocyanine as acceptor. This technol. is characterized by both a spectral selectivity and a temporal selectivity (due to the time-resolved mode), ensuring a highly specific signal. Here a europium-cryptate-labeled deoxyuridine **triphosphate** analog (K-11-dUTP) was used to monitor the extension reaction on a biotinylated oligonucleotide used as substrate for telomerase in a telomeric repeat amplification protocol (TRAP). After the addition of an allophycocyanine-streptavidin conjugate, the extension products give rise to a FRET between the incorporated cryptate moieties and the allophycocyanine acceptor that then displays a specific long-lived emission. The TRAP-HTRF format was validated as a screening tool by using a 2,6-diaminoanthraquinone analog, a known inhibitor of telomerase activity. The IC50 measured was consistent with the reported values, showing the convenience of the HTRF technol. for the study of telomerase activity and inhibitors.

CC 7-1 (Enzymes)  
 IT Oligonucleotides  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (biotinylated; homogeneous time-resolved **fluorescence**  
 detection of telomerase activity)  
 IT **Fluorescence** resonance energy transfer  
 (homogeneous time-resolved **fluorescence** detection of  
 telomerase activity)  
 IT 120178-12-3, Telomerase  
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
 study); BIOL (Biological study)  
 (homogeneous time-resolved **fluorescence** detection of  
 telomerase activity)  
 IT 213833-07-9, SA-XL 665 **221641-67-4**, K-11-UTP  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
 (Uses)  
 (homogeneous time-resolved **fluorescence** detection of  
 telomerase activity)  
 IT **221641-67-4**, K-11-UTP  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
 (Uses)  
 (homogeneous time-resolved **fluorescence** detection of  
 telomerase activity)  
 RN 221641-67-4 CAPLUS  
 CN Europate(2-), [10-[[[6-oxo-6-[[[(2E)-3-[1,2,3,4-tetrahydro-1-[5-O-  
 [hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-  
 ribofuranosyl]-2,4-dioxo-5-pyrimidinyl]-2-propenyl]amino]carbo  
 nyl]-1,14,39,40,41,42,43,44-octaazaocetacyclo[12.12.12.13,7.18,12.116,20.12  
 1,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,2  
 3,25(41),28,30,32(40),33,35,37(39)-octadecaene-5-carboxylato(5-)-  
 κN1,κN14,κN39,κN40,κN41,κN42,κN4  
 3,κN44]-, monohydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



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PAGE 3-A

● H<sup>+</sup>

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 18 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:730602 CAPLUS

DOCUMENT NUMBER: 142:149886

TITLE: Method for identifying neuronal cells suffering zinc toxicity by use of a novel fluorescent sensor

AUTHOR(S): Frederickson, Christopher J.; Burdette, Shawn C.; Frederickson, Cathy J.; Sensi, Stefano L.; Weiss, John H.; Yin, Hong Z.; Balaji, Rengarajan V.; Truong-Tran, Ai Q.; Bedell, Eric; Prough, Donald S.; Lippard, Stephen J.

CORPORATE SOURCE: NeuroBioTex, Inc., Galveston, TX, 77550, USA

SOURCE: Journal of Neuroscience Methods (2004), 139(1), 79-89  
CODEN: JNMEDT; ISSN: 0165-0270

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB During excitotoxic brain damage, injured neurons accumulate an anomalous, pathol. burden of weakly bound, rapidly exchangeable Zn<sup>2+</sup> that diffusely

fills the soma, nucleus and proximal dendrites. Mounting evidence indicates that this  $Zn^{2+}$  is a major contributing factor in the subsequent demise of the damaged neurons. Thus, identifying, imaging, and characterizing zinc-filled **cells** have become essential steps in understanding excitotoxicity. Here the authors demonstrate that a new **fluorescent** stain for zinc can rather selectively and quite vividly label zinc-filled neurons in frozen histol. sections. The method is more sensitive and selective than the existing stain TSQ, and simpler than the Timm-Danscher silver staining techniques. A previously unobserved population of apparently injured **cells** in the dentate gyrus has been discovered with the new reagent. Whereas **cells** viewed in situ in normal, healthy tissue virtually never display any perikaryal staining by histochem. methods for zinc [Histochem., 71 (1981) 1; Int. Rev. Neurobiol. 31 (1989) 145], injured **cells** stain intensely for zinc in culture [J. Neurosci. 17 (1997) 9554], acute slice preps. [J. Histochem. Cytochem. 47 (1999) 969; J. Neurosci. 22 (2002) 1273] and in tissue harvested in vivo [Science 272 (1996) 1013; Annu. Rev. Neurosci. 21 (1998) 347]. Thus, the presence of rapidly-exchangeable, "stainable" perikaryal zinc may be taken as an indicator of **cell** injury [J. Nutr. 130 (2000) 1471S; Biometals 14 (2001) 353].

CC 4-1 (Toxicology)

ST neuron zinc toxicity **fluorescent** sensor; **fluorescent** detection zinc neuron

IT Brain

(cortex; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT Brain

(dentate gyrus; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT Brain

(hippocampus; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT **Fluorescence**

**Fluorescence** microscopy

Neuron

Neurotoxicity

(method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT Brain

(neocortex, dorsal; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT Brain, disease

(trauma; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT 502467-23-4, Zinpyr 4

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

ANST (Analytical study); BIOL (Biological study); USES (Uses)

(Zinpyr 4; method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT 7440-66-6, Zinc, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)

(method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT 288574-78-7, Zinpyr-1

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

ANST (Analytical study); BIOL (Biological study); USES (Uses)

(method for identifying neuronal **cells** suffering zinc toxicity by use of a novel **fluorescent** sensor)

IT 288574-78-7, Zinpyr-1

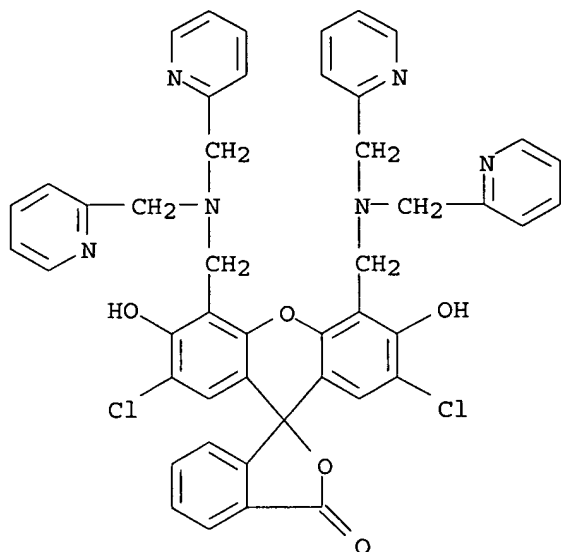
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);



ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (method for identifying neuronal cells suffering zinc  
 toxicity by use of a novel fluorescent sensor)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 19 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:643842 CAPLUS

DOCUMENT NUMBER: 141:342394

TITLE: Mono-, Bi-, and Trinuclear CuII-Cl Containing Products Based on the Tris(2-pyridylmethyl)amine Chelate Derived from Copper(I) Complex Dechlorination Reactions of Chloroform

AUTHOR(S): Lucchese, Baldo; Humphreys, Kristi J.; Lee, Dong-Heon; Incarvito, Christopher D.; Sommer, Roger D.; Rheingold, Arnold L.; Karlin, Kenneth D.

CORPORATE SOURCE: Department of Chemistry, The Johns Hopkins University, Baltimore, MD, 21218, USA

SOURCE: Inorganic Chemistry (2004), 43(19), 5987-5998  
 CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ligand TMPA (tris(2-pyridylmethyl)amine) and its copper complexes have played a prominent role in recent (bio)inorg. chemical studies; the copper(I) complex [CuI(TMPA)(CH3CN)]+ possesses an extensive dioxygen reactivity, and it is also known to effect the reductive dechlorination of substrates such as dichloromethane and benzyl and allyl chlorides. The authors describe a set of new analogs of TMPA, ligand 6TMPAOH (2-hydroxymethyl-6-(bis(2-pyridylmethyl)aminomethyl)pyridine), binucleating Iso-DO (bis(6-(bis(2-pyridylmethyl)aminomethyl)pyridin-2-yl)dimethyl ether), and trinucleating SYMM (tris(6-(bis(2-pyridylmethyl)aminomethyl)pyridin-2-

ylmethyl)amine). Copper(I) complexes with these ligands and a previously described binucleating ligand DO (bis(6-(bis(2-pyridylmethyl)aminomethyl)pyridin-3-yl)dimethyl ether) react with chloroform, resulting in reductive dechlorination and production of  $[\text{CuIIx}(\text{L})\text{Clx}]x^+$  ( $x = 1, 2, \text{ or } 3$ ). X-ray crystal structures of  $[\text{CuII}(\text{6TMPAOH})\text{Cl}]\text{PF}_6$ ,  $[\text{CuII}_2(\text{Iso-DO})\text{Cl}_2](\text{PF}_6)_2$ ,  $[\text{CuII}_2(\text{DO})\text{Cl}_2](\text{PF}_6)_2$ , and  $[\text{CuII}_3(\text{SYMM})\text{Cl}_3](\text{PF}_6)_3$  are presented, and the compds. are also characterized by UV-visible and EPR spectroscopies as well as cyclic voltammetry. The steric influence of a pyridyl 6-substituent (in the complexes with 6TMPAOH, Iso-DO, and SYMM) on the solid state and solution structures and redox potentials are compared and contrasted to those chlorocopper(II) complexes with a pyridyl 5'-substituent (in  $[\text{CuII}_2(\text{DO})\text{Cl}_2](\text{PF}_6)_2$  and in  $[\text{CuII}(\text{TMPA})\text{Cl}]^+$ ). Some insights into the reductive dechlorination process were obtained by using  $^2\text{H}$  NMR spectroscopy in following the reaction of  $[\text{Cu}_2(\text{Iso-DO})(\text{CH}_3\text{CN})_2](\text{PF}_6)_2$  with  $\text{CDCl}_3$ , in the presence or absence of a radical trap, 2,4-di-tert-butylphenol.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 72, 75

IT 769952-14-9P 770722-09-3P 770723-00-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal and mol. structure)

IT 769952-13-8P 770722-65-1P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and cyclic voltammetry)

IT 1539-42-0, Bis(2-picoly)amine 3099-28-3, 2,6-Bis(chloromethyl)pyridine 14057-91-1, Tetrakis(acetonitrile)copper(1+) perchlorate 64443-05-6, Tetrakis(acetonitrile)copper(1+) **hexafluorophosphate** 175858-94-3 769952-03-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of copper acetonitrile and chloro mono-, bi- and trinuclear complexes of chelates based on tris(pyridylmethyl)amine)

IT 279216-08-9P 279216-12-5P 769951-98-6P 769951-99-7P 769952-00-3P 769952-01-4P 769952-02-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of copper acetonitrile and chloro mono-, bi- and trinuclear complexes of chelates based on tris(pyridylmethyl)amine)

IT 769952-05-8P 769952-07-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of copper acetonitrile and chloro mono-, bi- and trinuclear complexes of chelates based on tris(pyridylmethyl)amine)

IT 769952-14-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal and mol. structure)

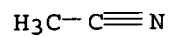
RN 769952-14-9 CAPLUS

CN Copper(3+),  $[\mu_3\text{-}[\text{N,N-bis}[[6\text{-}[[\text{bis}[(2\text{-pyridinyl-}\kappa\text{N})\text{methyl}]\text{amino-}\kappa\text{N})\text{methyl}]\text{-2-pyridinyl-}\kappa\text{N})\text{methyl}]\text{-N',N'-bis}[(2\text{-pyridinyl-}\kappa\text{N})\text{methyl}]\text{-2,6-pyridinedimethanamine-}\kappa\text{N1},\kappa\text{N2}]]\text{trichlorotri-}, \text{tris}[\text{hexafluorophosphate}(1-)]$ , compd. with acetonitrile (1:1) (9CI)  
(CA INDEX NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 769952-13-8

CMF C57 H57 Cl3 Cu3 N13 . 3 F6 P

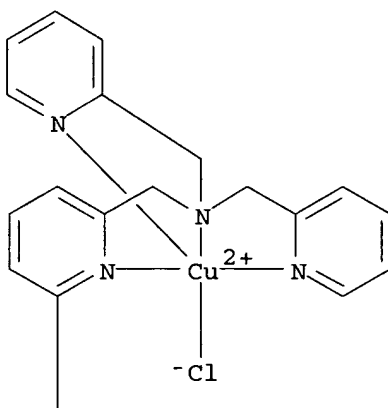
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CRN 769952-12-7

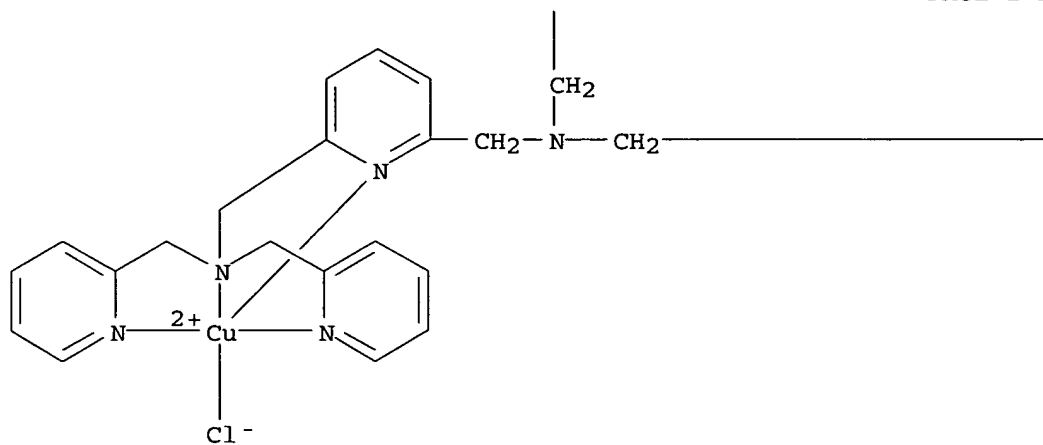
CMF C57 H57 Cl3 Cu3 N13

CCI CCS

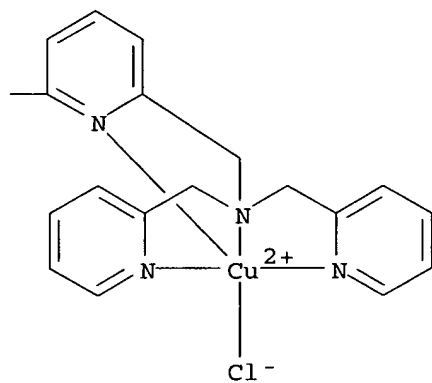
PAGE 1-A



PAGE 2-A



PAGE 2-B

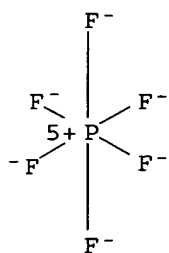


CM 4

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 769952-13-8P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and cyclic voltammetry)

RN 769952-13-8 CAPLUS

CN Copper(3+),  $[\mu_3 - [N,N\text{-bis}[[6 - [bis[(2\text{-pyridinyl-}\kappa N)\text{methyl}]\text{amino-}\kappa N]\text{methyl}]\text{-}2\text{-pyridinyl-}\kappa N]\text{methyl}]\text{-}N',N'\text{-bis}[(2\text{-pyridinyl-}\kappa N)\text{methyl}]\text{-}2,6\text{-pyridinedimethanamine-}\kappa N1,\kappa N']]\text{trichlorotri-}, \text{tris}[\text{hexafluorophosphate}(1-)]$  (9CI) (CA INDEX NAME)

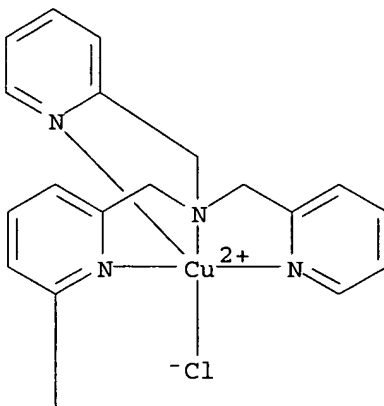
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CRN 769952-12-7

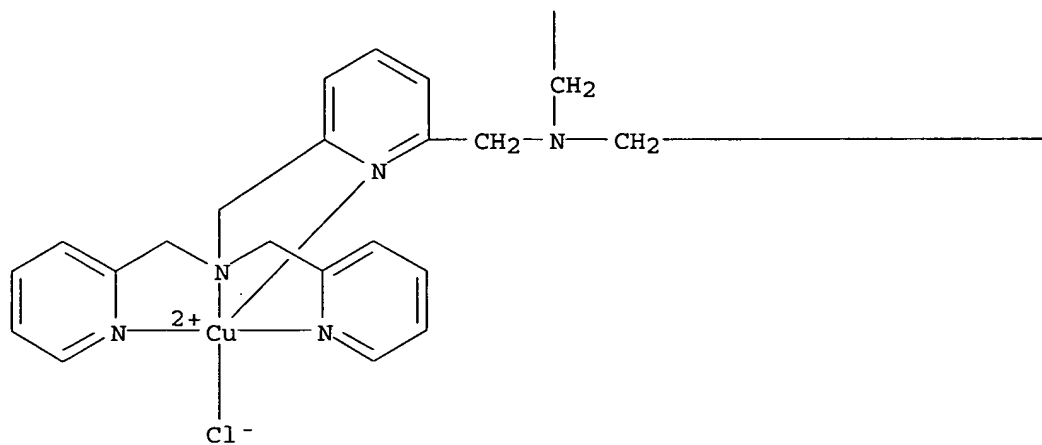
CMF C57 H57 Cl3 Cu3 N13

CCI CCS

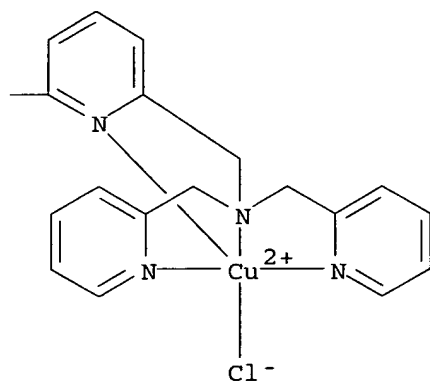
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PAGE 2-A



PAGE 2-B

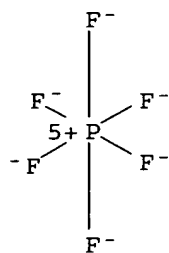


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

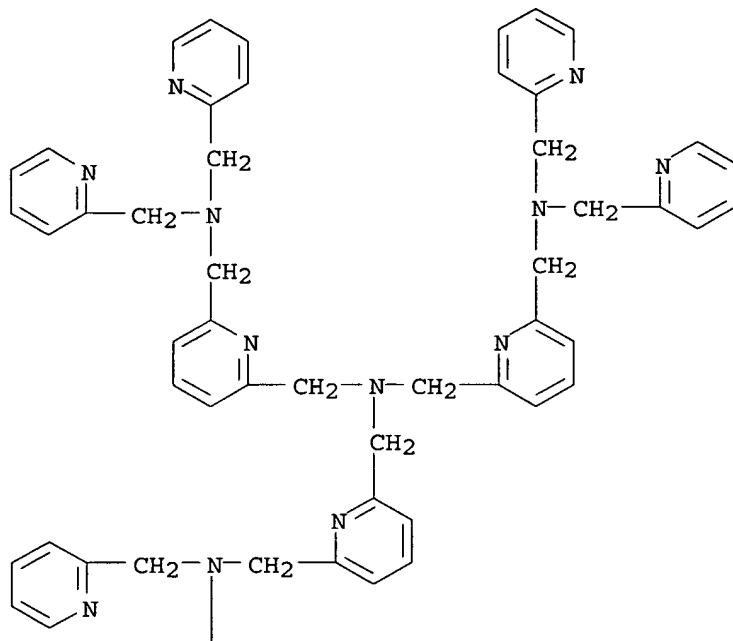


IT 769952-02-5P

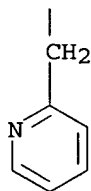
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of copper acetonitrile and chloro mono-, bi- and trinuclear complexes of chelates based on tris(pyridylmethyl)amine)

RN 769952-02-5 CAPLUS  
 CN 2,6-Pyridinedimethanamine, N,N-bis[[6-[[bis(2-pyridinylmethyl)amino]methyl]-2-pyridinyl]methyl]-N',N'-bis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

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IT 769952-07-0P

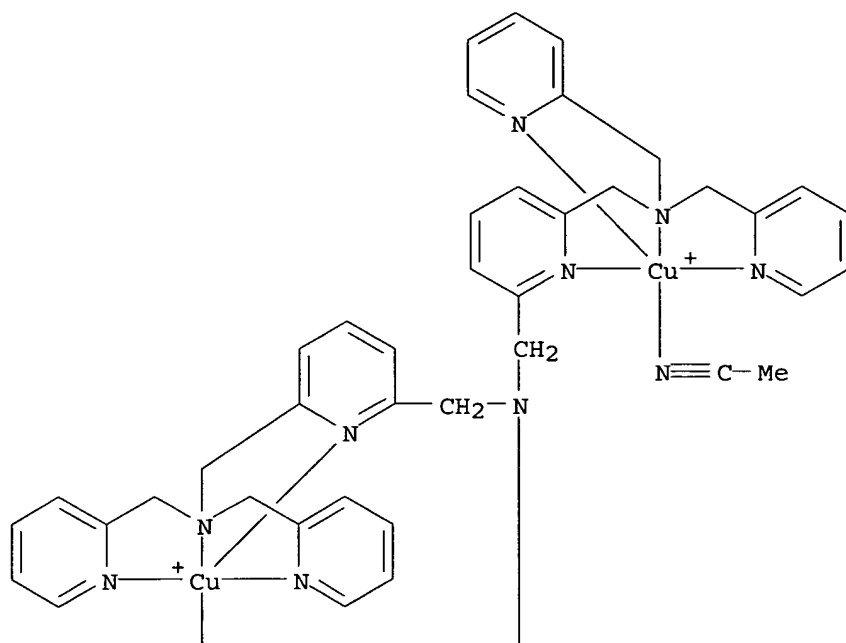
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of copper acetonitrile and chloro mono-, bi- and trinuclear complexes of chelates based on tris(pyridylmethyl)amine)

RN 769952-07-0 CAPLUS  
 CN Copper(3+), tris(acetonitrile) [μ3-[N,N-bis[[6-[[bis[(2-pyridinyl-κN)methyl]amino-κN)methyl]-2-pyridinyl-κN)methyl]-N',N'-bis[(2-pyridinyl-κN)methyl]-2,6-pyridinedimethanamine-κN1,κN']]tri-, tris[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

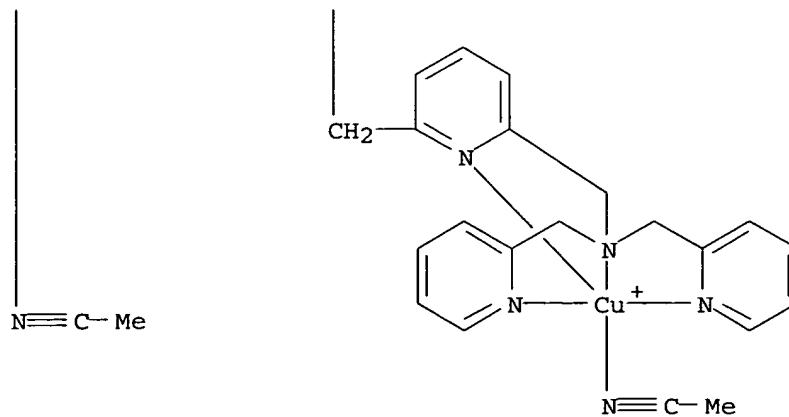
CM 1

CRN 769952-06-9  
CMF C63 H66 Cu3 N16  
CCI CCS

PAGE 1-A



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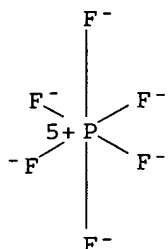


CM 2

CRN 16919-18-9



CMF F6 P  
CCI CCS



REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 20 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:480782 CAPLUS

DOCUMENT NUMBER: 142:399829

TITLE: Spectroscopic behavior of hybrid materials obtained by the sol-gel technique

AUTHOR(S): Sokolnicki, J.; Wiglusz, R.; Radzki, S.; Graczyk, A.; Legendziewicz, J.

CORPORATE SOURCE: Faculty of Chemistry, University of Wroclaw, Wroclaw, 50-383, Pol.

SOURCE: Optical Materials (Amsterdam, Netherlands) (2004), 26(2), 199-206

CODEN: OMATET; ISSN: 0925-3467

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The need for new, chemical and phys. stable luminescent materials operating with UV excitations has stimulated research on luminescence properties of doped sol-gel material. In this work we present the technol. of production of silica gels doped with organic mols., lanthanide compds., and organic/inorg. composites. Optical properties of these materials as functions of temperature, concentration, and excitation wavelength are presented. Dynamics of the excited

states is discussed based on the decay times and emission efficiencies data. Mechanisms of ligand-to-metal energy transfer as well as other processes affecting emission efficiency are considered. Silica sol-gels doped with di-amino acid derivs. of porphyrins: PP(Ser)2(Arg)2, PP(Ala)2(Arg)2, PP(Met)2(Arg)2, where Met, Arg, and Ser denote methionine, **serine**, and arginine amino acids, resp., and H2TMePP {tetrakis[4-(trimethylammonio)phenyl]-21H,23H-porphine} have been obtained and spectroscopically studied. The samples emit only from the lowest excited singlet state (S1). The intensity of this emission depends on the concentration of the active mol. and time of the exposition to the excitation beam. The sample containing PP(Ser)2(Arg)2 co-doped with Tb(III) ions exhibits only 5D4 emission from the metal center. When co-doped with Pr(III) ions, it displays only the S1 emission and the metal ions affect the S2 → S1 internal conversion. These materials can find applications as **phosphors** or sensors of UV irradiation. Efforts have been undertaken also to obtain chiral anisotropic materials.

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 66, 78

IT 69458-20-4 188014-02-0 849771-18-2 849771-20-6 849771-22-8

849771-23-9

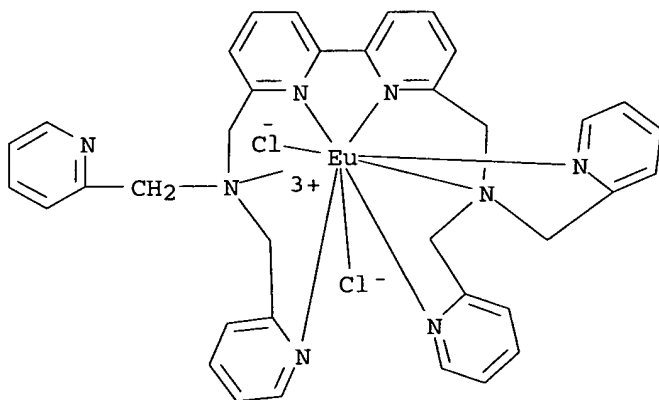
RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)  
 (luminescence of hybrid materials of silica gels doped with organic mols.  
 or lanthanide compds. obtained by the sol-gel technique)

IT 188014-02-0 849771-23-9

RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)  
 (luminescence of hybrid materials of silica gels doped with organic mols.  
 or lanthanide compds. obtained by the sol-gel technique)

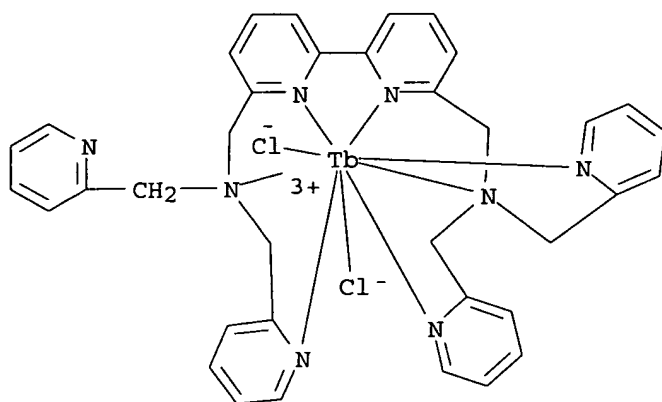
RN 188014-02-0 CAPLUS

CN Europium(1+), dichloro[N,N,N'-tris[(2-pyridinyl-κN)methyl]-N'-(2-pyridinylmethyl) [2,2'-bipyridine]-6,6'-dimethanamine-κN1,κN1',κN6,κN6']-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

RN 849771-23-9 CAPLUS

CN Terbium(1+), dichloro[N,N,N'-tris[(2-pyridinyl-κN)methyl]-N'-(2-pyridinylmethyl) [2,2'-bipyridine]-6,6'-dimethanamine-κN1,κN1',κN6,κN6']-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 21 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:274844 CAPLUS

DOCUMENT NUMBER: 141:63818

TITLE: Strain-induced substitutional lability in a Ru(II) complex of a hypodentate polypyridine ligand

AUTHOR(S): Akermark, Bjoern; Bjernemose, Jens; Boerje, Anna; Chmielewski, Piotr J.; Paulsen, Hauke; Simonsen, Ole; Stein, Paul C.; Toftlund, Hans; Wolny, Juliusz A.

CORPORATE SOURCE: Stockholms Universitet, Stockholm, 106 91, Swed.

SOURCE: Dalton Transactions (2004), (8), 1215-1220

CODEN: DTARAF; ISSN: 1477-9226

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:63818

AB The Ru(II) complex of heptadentate N,N,N',N'-tetrakis(2-pyridylmethyl)-2,6-bis(aminomethyl)pyridine (tpap) was isolated as the hexafluorophosphate complex Ru(tpap)(PF<sub>6</sub>)<sub>2</sub>. The crystal structure was determined for the triflate salt Ru(tpap)(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>·2H<sub>2</sub>O, which crystallizes in the monoclinic space group P2<sub>1</sub>/n. The structure was refined to a final R value of 0.0549 for 5894 observed reflections. The heptadentate ligand coordinates with six nitrogens, i.e. with two tertiary nitrogens and four pyridine nitrogens, one of the pyridines remaining un-coordinated. The resulting structure is significantly distorted from octahedral geometry with an equatorial Nsp<sup>3</sup>-Ru-Npyridine angle of 120°. The consequence of the above steric strain is a labilization of the system and fluxional behavior involving exchange between equatorially coordinated and noncoordinated pyridines was observed by <sup>1</sup>H NMR for Ru(tpap)(PF<sub>6</sub>)<sub>2</sub> in d<sub>6</sub>-acetone solution. The activation parameters of ΔG<sup>‡</sup><sub>298</sub> = 53 kJ mol<sup>-1</sup>, ΔH<sup>‡</sup> = 56 ± 1 kJ mol<sup>-1</sup> and ΔS<sup>‡</sup> = -10 ± 3 J mol<sup>-1</sup> K<sup>-1</sup> were determined from NMR expts. In addition electronic structure calcns. applying d. functional theory (DFT) were performed to identify a transition state and to estimate the activation barrier. From NMR and DFT results the mechanism of isoexchange involving a heptacoordinated intermediate is proposed.

CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 27, 67, 75

IT 495417-60-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (Strain-induced substitutional lability in a Ru(II) complex of a  
 hypodentate polypyridine ligand)

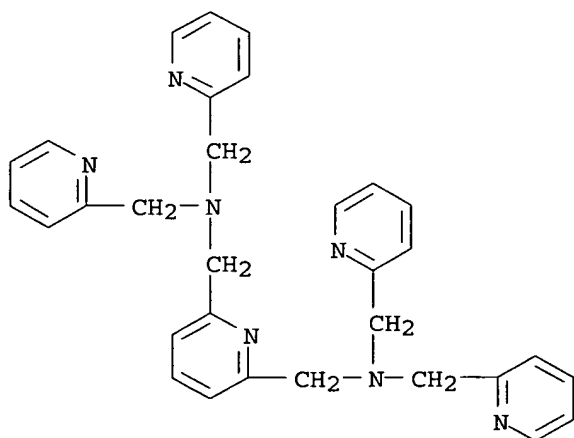
IT 708986-49-6P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)

IT 708986-47-4P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical  
 process); PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation); PROC (Process)  
 (preparation and kinetics of fluxional rearrangement of)

IT 495417-60-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (Strain-induced substitutional lability in a Ru(II) complex of a  
 hypodentate polypyridine ligand)

RN 495417-60-2 CAPLUS

CN 2,6-Pyridinedimethanamine, N,N,N',N'-tetrakis(2-pyridinylmethyl)- (9CI)  
 (CA INDEX NAME)



IT 708986-49-6P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)

RN 708986-49-6 CAPLUS

CN Ruthenium(2+), [N,N,N'-tris[(2-pyridinyl-κN)methyl]-N'-(2-  
 pyridinylmethyl)-2,6-pyridinedimethanamine-κN1,κN2,κN6]-  
 , (OC-6-24)-, salt with trifluoromethanesulfonic acid (1:2), monohydrate  
 (9CI) (CA INDEX NAME)

CM 1

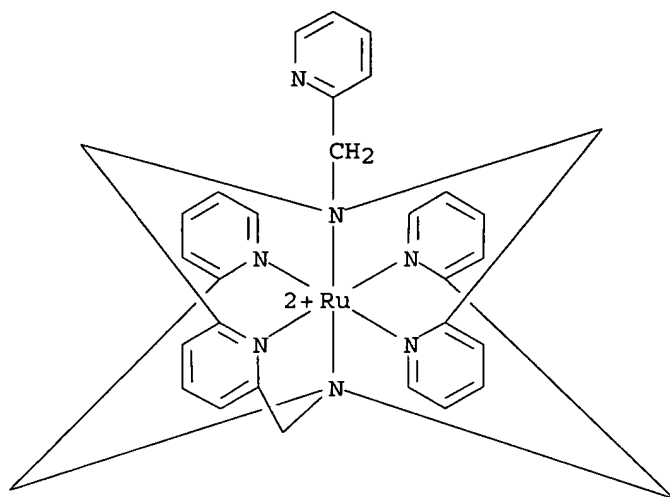
CRN 708986-48-5

CMF C31 H31 N7 Ru . 2 C F3 O3 S

CM 2

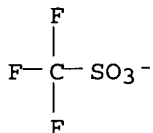
CRN 708986-46-3

CMF C31 H31 N7 Ru  
CCI CCS



CM 3

CRN 37181-39-8  
CMF C F3 O3 S



IT 708986-47-4P

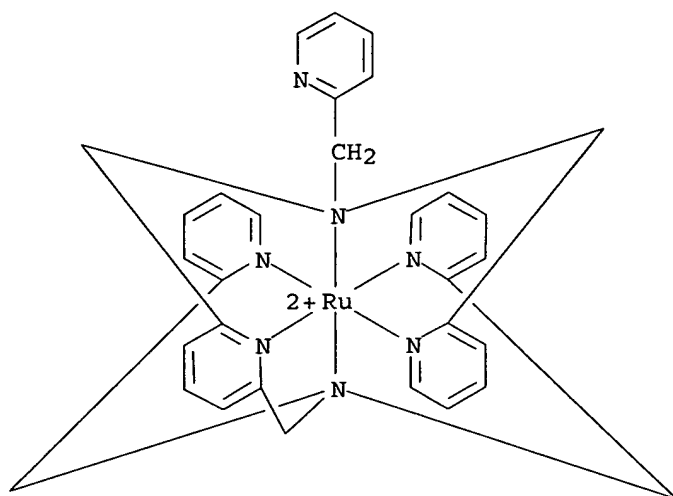
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and kinetics of fluxional rearrangement of)

RN 708986-47-4 CAPLUS

CN Ruthenium(2+), [N,N,N'-tris[(2-pyridinyl-κN)methyl]-N'-(2-pyridinylmethyl)-2,6-pyridinedimethanamine-κN1,κN2,κN6]-, (OC-6-24)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 708986-46-3  
CMF C31 H31 N7 Ru  
CCI CCS

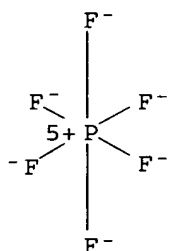


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 22 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:596998 CAPLUS

DOCUMENT NUMBER: 139:288426

TITLE: Cross-linking strategy for molecular recognition and fluorescent sensing of a multi-phosphorylated peptide in aqueous solution

AUTHOR(S): Ojida, Akio; Inoue, Masaaki; Mitooka, Yasuko; Hamachi, Itaru

CORPORATE SOURCE: Institute for Materials Chemistry and Engineering (IMCE) and Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, PRESTO (Organization and Function JST), Fukuoka, 812-8581, Japan

SOURCE: Journal of the American Chemical Society (2003), 125(34), 10184-10185

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB In the research field of mol. recognition, selective recognition and sensing of **phosphorylated** protein surfaces is strongly desirable both for elucidation of protein-protein recognition at the mol. level and for regulation of signal transduction through protein surfaces. Here we describe a new strategy for mol. recognition of a multi-**phosphorylated** peptide using intrapeptide crosslinking on the basis of coordination chemical. The present artificial receptor can selectively bind to doubly **phosphorylated** peptide through multiple-point interactions and **fluorescently** sense the binding event with an association constant of more than  $10^6$  M<sup>-1</sup> in neutral aqueous solution

CC 9-5 (Biochemical Methods)  
 Section cross-reference(s): 79, 80

ST cross linking mol recognition **fluorescence** sensor

IT **Fluorometry**  
 Molecular recognition  
 (crosslinking strategy for mol. recognition and **fluorescent** sensing of multi-**phosphorylated** peptide in aqueous solution)

IT Peptides, analysis  
 RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); ANST (Analytical study); PROC (Process)  
 (crosslinking strategy for mol. recognition and **fluorescent** sensing of multi-**phosphorylated** peptide in aqueous solution)

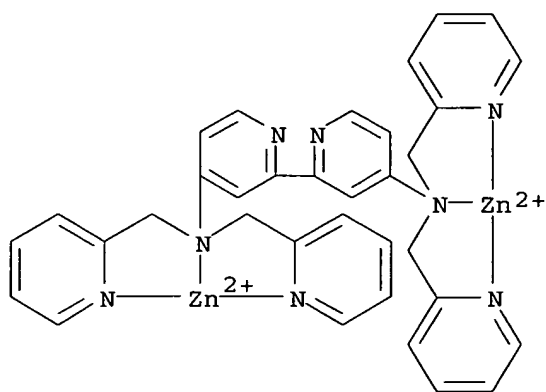
IT Sensors  
 (**fluorescence** chemo; crosslinking strategy for mol. recognition and **fluorescent** sensing of multi-**phosphorylated** peptide in aqueous solution)

IT 607729-62-4 607729-63-5 607729-64-6 607729-65-7 607729-66-8  
 607729-67-9 607729-68-0 **608125-15-1 608125-16-2**  
**608125-17-3** 608125-18-4 608125-19-5  
 RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); ANST (Analytical study); PROC (Process)  
 (crosslinking strategy for mol. recognition and **fluorescent** sensing of multi-**phosphorylated** peptide in aqueous solution)

IT **608125-15-1 608125-16-2 608125-17-3**  
 RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); ANST (Analytical study); PROC (Process)  
 (crosslinking strategy for mol. recognition and **fluorescent** sensing of multi-**phosphorylated** peptide in aqueous solution)

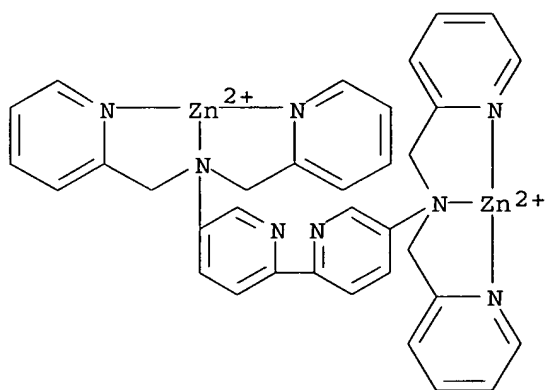
RN 608125-15-1 CAPLUS

CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl][2,2'-bipyridine]-4,4'-diamine- $\kappa$ N4: $\kappa$ N4']]di- (9CI) (CA INDEX NAME)



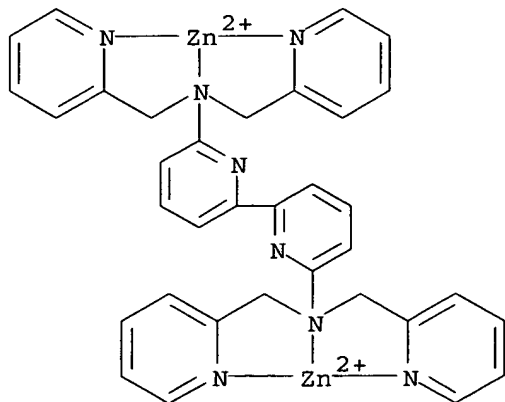
RN 608125-16-2 CAPLUS

CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl][2,2'-bipyridine]-5,5'-diamine- $\kappa$ N5: $\kappa$ N5']]di- (9CI) (CA INDEX NAME)



RN 608125-17-3 CAPLUS

CN Zinc(4+), [ $\mu$ -[N,N,N',N'-tetrakis[(2-pyridinyl- $\kappa$ N)methyl][2,2'-bipyridine]-6,6'-diamine- $\kappa$ N6: $\kappa$ N6']]di- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 23 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003/290931 CAPLUS  
 DOCUMENT NUMBER: 139/145971  
 TITLE: A macrocyclic zinc(II) **fluorophore** as a detector of apoptosis  
 AUTHOR(S): Kimura, Eiichi; Aoki, Shin; Kikuta, Emiko; Koike, Tohru  
 CORPORATE SOURCE: Faculty of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima, 739-8521, Japan  
 SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2003), 100(7), 3731-3736  
 CODEN: PNASA6; ISSN: 0027-8424  
 PUBLISHER: National Academy of Sciences  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Our originally designed dansylamidoethylcyclen 4 as a biomimetic Zn<sup>2+</sup>-selective **fluorophore** has been demonstrated to be a good detector of the apoptosis (induced by an anticancer agent, etoposide, and H<sub>2</sub>O<sub>2</sub>) in cancer **cells** such as HeLa and HL60 **cells**. The macrocyclic Zn<sup>2+</sup> ligand 4 (mostly as a deprotonated form) is **cell**-permeable to show weak **fluorescence** (emission at 550 nm), which forms a strong **fluorescent** 1:1 Zn<sup>2+</sup> complex 5 (emission at 530 nm) when Zn<sup>2+</sup> is incorporated into the **cells** by a zinc(II) ionophore pyrithione. Thus formed, Zn<sup>2+</sup> complex 5 is **cell**-impermeable and remains intact over a few hours. When apoptosis in HeLa or HL60 **cells** is artificially induced, 4 selectively and strongly stains apoptotic **cells** only at early stages, which was verified by using the conventional apoptotic detection probe annexin V-Cy3. Detection of the apoptotic **cells** by 4 was perhaps due to significantly increased free Zn<sup>2+</sup> flux at early stages of apoptosis. Apoptotic detection by 4 has been compared with a presently available Zn<sup>2+</sup> **fluorophore**, Zinquin. We present that 4 has advantages in detection of apoptosis over annexin V-Cy3 and Zinquin.

CC 9-4 (Biochemical Methods)  
 Section cross-reference(s): 14

ST macrocyclic zinc **fluorophore** detector apoptosis

IT Annexins  
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
 (V; macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT Antitumor agents  
 (apoptosis induced by; macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT Apoptosis  
 Biological transport  
**Fluorescence** microscopy  
**Fluorescent** substances  
 Human  
 Neoplasm  
 Staining, biological  
 (macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT 7722-84-1, Hydrogen peroxide, biological studies 33419-42-0, Etoposide  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (apoptosis induced by; macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT 146368-16-3, Cy3 181530-09-6  
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)

(macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT 16858-02-9, TPEN 20214-91-9D, Zinc2, reaction with zinquin, biological studies 23713-49-7, Zinc(II), biological studies 61864-80-0 151606-29-0 151606-29-0D, reaction with zinc 184537-04-0 209547-49-9 **288574-78-7**, Zinpyr-1 569654-63-3

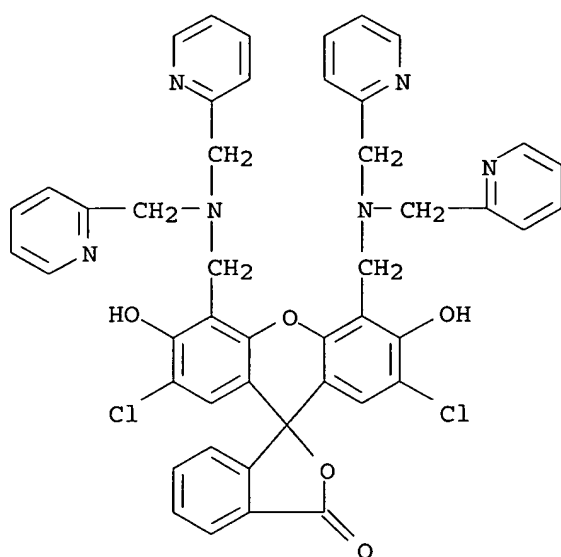
RL: BSU (Biological study, unclassified); BIOL (Biological study) (macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

IT **288574-78-7**, Zinpyr-1

RL: BSU (Biological study, unclassified); BIOL (Biological study) (macrocyclic zinc(II) **fluorophore** as detector of apoptosis)

RN 288574-78-7 CAPLUS

CN Spiro[isobenzofuran-1(3H), 9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 24 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:859295 CAPLUS

DOCUMENT NUMBER: 137:381830

TITLE: Naked-eye detection of **phosphate** ions in water at physiological pH. A remarkably selective and easy-to-assemble colorimetric **phosphate**-sensing probe

AUTHOR(S): Han, Min Su; Kim, Dong H.

CORPORATE SOURCE: Center for Integrated Molecular Systems, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Angewandte Chemie, International Edition (2002), 41(20), 3809-3811

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

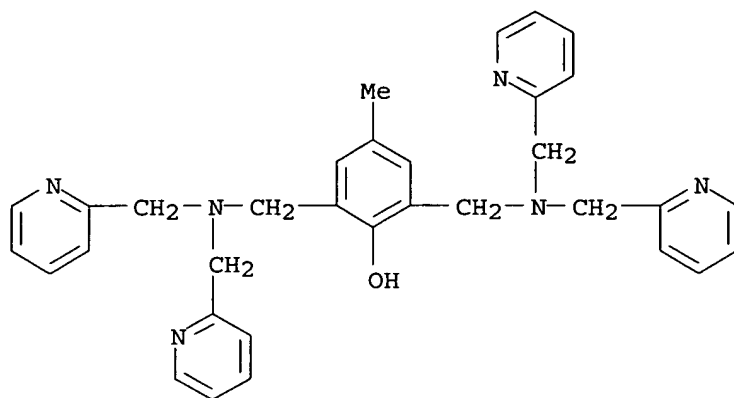
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A colorimetric sensor was developed that allows the detection of **phosphate** anions in aqueous solns. at neutral pH values. The sensor

was assembled based on metal-ligand interactions by mixing 2,6-bis(bis(2-pyridylmethyl)aminomethyl)-4-methylphenol (H-bpmp) and Zn perchlorate to form a receptor complex and further mixing with pyrocatechol violet as pH sensitive dye in an aqueous buffer solution of pH 7. The solution had a blue color ( $\lambda_{\text{max}}=624$  nm) ascribed to the binding of pyrocatechol violet to form  $[\text{Zn}_2(\text{H-bpmp})(\text{pyrocatechol violet})]^{+}$ . The addition of **phosphate** anions to this solution resulted in a change of color to yellow. Thermodyn. parameters and association consts. showed that **phosphate** bound to the receptor over 2-fold more tightly than the indicator. The sensor had a high selectivity for **phosphate** with regard to other anions as sulfate or **fluoride** ions. The use of the sensor for the naked-eye **phosphate** detection is demonstrated.

- CC 9-5 (Biochemical Methods)  
Section cross-reference(s): 79
- ST **phosphate** sensor colorimetry physiol pH
- IT Colorimetry  
Optical sensors  
pH  
(naked-eye detection of **phosphate** ions in water at physiol. pH)
- IT Enthalpy  
Entropy  
Free energy  
(naked-eye detection of **phosphate** ions in water at physiol. pH in relation to)
- IT 7365-45-9, Hepes  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(buffer; naked-eye detection of **phosphate** ions in water at physiol. pH using)
- IT 14265-44-2, **Phosphate**, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(naked-eye detection of **phosphate** ions in water at physiol. pH)
- IT 115-41-3, Pyrocatechol violet 13637-61-1, Zinc perchlorate  
**80528-41-2**, 2,6-Bis(bis(2-pyridylmethyl)aminomethyl)-4-methylphenol  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(naked-eye detection of **phosphate** ions in water at physiol. pH using)
- IT **80528-41-2**, 2,6-Bis(bis(2-pyridylmethyl)aminomethyl)-4-methylphenol  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(naked-eye detection of **phosphate** ions in water at physiol. pH using)
- RN 80528-41-2 CAPLUS
- CN Phenol, 2,6-bis[[bis(2-pyridinylmethyl)amino]methyl]-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 25 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:645580 CAPLUS

DOCUMENT NUMBER: 138:316954

TITLE: Homogeneous **Phosphodiesterase** and Hybridization Assays Using Europium Cryptate: Oligonucleotide Conjugates

AUTHOR(S): Bazin, H.; Guillemer, S.; Mathis, G.

CORPORATE SOURCE: HTRF Bioassays, CIS Bio International, Bagnols sur Ceze, F-30 204, Fr.

SOURCE: Journal of Fluorescence (2002), 12(2), 245-248

CODEN: JOFLEN; ISSN: 1053-0509

PUBLISHER: Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Upon conjugation to single-stranded oligonucleotides, a europium cryptate ( $\text{Eu}^{3+}$  + tris-bipyridine) showed a marked increase in its **fluorescence** lifetime and was much less sensitive to **fluorescence** quenching by uric acid. This behavior was shown to be moderately dependent on the length and sequence of the oligonucleotide and all the single-stranded oligonucleotides studied displayed similar behavior. In contrast, a cryptate moiety attached to a double-stranded oligonucleotide did not display such an increase in its **fluorescence** lifetime and was quenched in presence of uric acid. Taking advantage of this unique behavior characterizing single-stranded K-ODN conjugates, a new concept of dosage based on the modulation of the cryptate **fluorescence** by a quencher was set up. This **fluorescence** quenching assay involving a single **fluorescent** label was applied to the monitoring of hybridization reactions and detection of a **phosphodiesterase** activity.

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 6

ST nucleic acid hybridization **phosphodiesterase** assay europium cryptate oligonucleotide conjugate

IT Nucleic acid hybridization

(assay; homogeneous **phosphodiesterase** and hybridization assays using europium cryptate oligonucleotide conjugates)

IT Oligonucleotides

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

ANST (Analytical study); BIOL (Biological study); USES (Uses)

(conjugates; homogeneous **phosphodiesterase** and hybridization

assays using europium cryptate oligonucleotide conjugates)

IT **Fluorescence**  
**Fluorescence** quenching  
(homogeneous **phosphodiesterase** and hybridization assays using  
europium cryptate oligonucleotide conjugates)

IT 9025-82-5, **Phosphodiesterase**  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(assay; homogeneous **phosphodiesterase** and hybridization  
assays using europium cryptate oligonucleotide conjugates)

IT 125433-96-7 509154-67-0 510776-22-4 510776-23-5  
510776-24-6 510776-25-7 510776-26-8 510776-27-9 510776-28-0  
510776-29-1 511313-41-0  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(homogeneous **phosphodiesterase** and hybridization assays using  
europium cryptate oligonucleotide conjugates)

IT 7440-53-1, Europium, biological studies  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(homogeneous **phosphodiesterase** and hybridization assays using  
europium cryptate oligonucleotide conjugates)

IT 125433-96-7  
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);  
ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(homogeneous **phosphodiesterase** and hybridization assays using  
europium cryptate oligonucleotide conjugates)

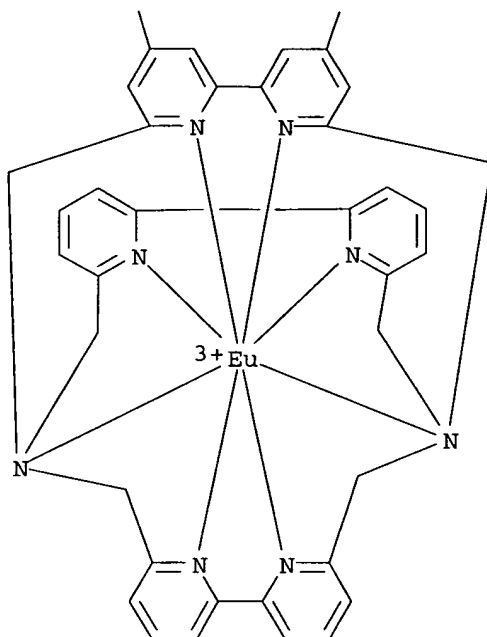
RN 125433-96-7 CAPLUS

CN Europium(3+), [N,N'-bis(2-aminoethyl)-1,14,39,40,41,42,43,44-  
octaazaocetacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetr  
aconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,  
37(39)-octadecaene-5,10-dicarboxamide-N1,N14,N39,N40,N41,N42,N43,N44]-  
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



## REFERENCE COUNT:

7/2 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 26 OF 52

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

AB Di- or trinuclear Cu(II) complexes efficiently catalyzed the condensation  
of glycine with formaldehyde to yield **serine** at pH 7.3,  
50°.

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 78

ST **serine** prepn glycine reaction formaldehyde copper complex  
catalyst

IT Reaction mechanism

(reaction of glycine with formaldehyde to give **serine** in the  
presence of copper-based catalysts in neutral aqueous solution)

IT Amino acids, reactions